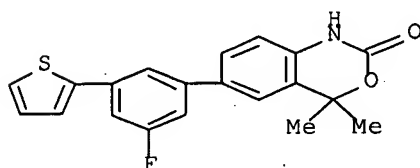
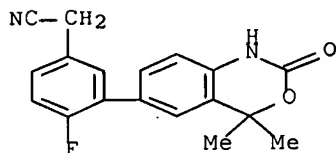


RN 305839-71-8 CAPLUS
 CN 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(2-thienyl)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

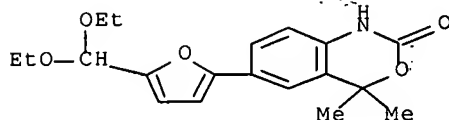


*Method of making
compound claim*

RN 305839-75-2 CAPLUS
 CN Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro- (9CI) (CA INDEX NAME)



RN 305839-76-3 CAPLUS
 CN 2H-3,1-Benzoxazin-2-one, 6-[5-(diethoxymethyl)-2-furanyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:790488 CAPLUS Full-text
 DOCUMENT NUMBER: 133-350228

TITLE: Preparation of cyclothiocarbamate derivatives as *obru* progesterone receptor modulators

INVENTOR(S): Zhang, Puwen; Fensome, Andrew;
 Terefenko, Eugene A.; Zhi, Lin;
 Jones, Todd K.; Marschke, Keith B.;
 Tegley, Christopher M.

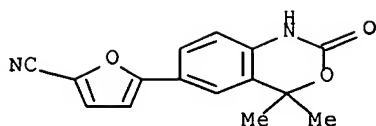
PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 101 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

*(document
is not available)*



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

125 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:669675 CAPLUS Full-text

DOCUMENT NUMBER: 137:201317

TITLE: Preparation of benzoxazinone cyclic carbamate
antiproggestins for use in combination therapies and
regimens with progestational agents.

INVENTOR(S): Grubb, Gary S.; Zhang, Puwen;
Terefenko, Eugene A.; Fensome, Andrew
; Wrobel, Jay E.; Fletcher, Iii Horace;
Edwards, James P.; Jones, Todd K.;
Tegley, Christopher M.; Zhi, Lin

PATENT ASSIGNEE(S): Wyeth, John and Brother Ltd., USA; Ligand
Pharmaceuticals Incorporated

SOURCE: U.S., 44 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent
LANGUAGE: English

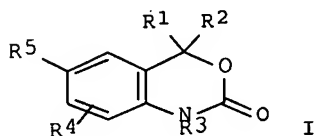
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6444668	B1	20020903	US 2000-552350	20000419
CA 2372773	A1	20001109	CA 2000-2372773	20000501
JP 2002543155	T	20021217	JP 2000-615048	20000501
AT 275973	T	20041015	AT 2000-928611	20000501
PT 1173210	T	20050131	PT 2000-928611	20000501
ES 2226833	T3	20050401	ES 2000-928611	20000501
MX 2001PA11311	A	20030714	MX 2001-PA11311	20011105
US 2003045511	A1	20030306	US 2002-141792	20020509
US 6759408	B2	20040706		
HK 1043736	A1	20050401	HK 2002-104868	20020628
PRIORITY APPLN. INFO.:			US 1999-229346P	P 19990504
			US 1999-304712	A 19990504
			US 2000-552350	A 20000419
			WO 2000-US11643	W 20000501

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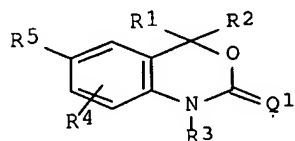
OTHER SOURCE(S): MARPAT 137:201317
GI



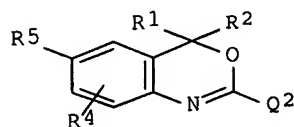
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066570	A1	20001109	WO 2000-US11749	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6436929	B1	20020820	US 2000-552354	20000419
CA 2371712	A1	20001109	CA 2000-2371712	20000501
EP 1175411	A1	20020130	EP 2000-930266	20000501
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010214	A	20020213	BR 2000-10214	20000501
TR 200103285	T2	20020221	TR 2001-3285	20000501
JP 2002543192	T	20021217	JP 2000-615600	20000501
HU 200203332	A2	20030128	HU 2002-3332	20000501
AU 766801	B2	20031023	AU 2000-48119	20000501
CN 1131856	B	20031224	CN 2000-807099	20000501
NZ 515353	A	20040326	NZ 2000-515353	20000501
SG 120970	A1	20060426	SG 2004-81	20000501
ZA 2001007633	A	20020514	ZA 2001-7633	20010917
IN 2001MN01294	A	20050304	IN 2001-MN1294	20011018
NO 2001005381	A	20020103	NO 2001-5381	20011102
NO 321370	B1	20060502		
BG 106080	A	20020531	BG 2001-106080	20011102
MX 2001PA11287	A	20030714	MX 2001-PA11287	20011105
US 2003092711	A1	20030515	US 2002-140034	20020506
US 7081457	B2	20060725		
US 2006142280	A1	20060629	US 2006-351002	20060209
PRIORITY APPLN. INFO.:			US 1999-183013P	P 19990504
			US 2000-552354	A1 20000419
			WO 2000-US11749	W 20000501
			US 2002-140034	A3 20020506

OTHER SOURCE(S):
GI

MARPAT 133:350228



I



II

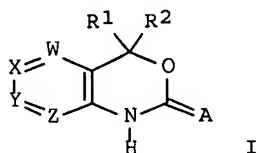
AB The title compds. [I or II; R1, R2 = H, alkyl, alkenyl, etc.; or R1 and R2 are fused to form (un)substituted 3-8 membered spiro cyclic alkyl or alkenyl ring or a spiro cyclic ring containing 1-3 heteroatoms selected from O, S and N; R3 = H, OH, NH2, etc.; R4 = H, halo, CN, etc.; R5 = (un)substituted Ph, 5-6 membered heterocyclic ring with 1-3 ring heteroatoms, 3-pyridyl, 5-pyrimidinyl; Q1 = S, NR7, CR8R9; R7 = CN, alkyl, cycloalkyl, etc.; R8, R9 = H, alkyl, cycloalkyl, etc.; Q2 = NR11OR12, NR11NR12R13, ONR11R13; R11-R13 = H, alkyl, aryl, etc.] which are agonists of the progesterone receptor, and are useful for contraception and the treatment of progesterone-related maladies,

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 15 OF 26 MARPAT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 128:282840 MARPAT Full-text
 TITLE: Preparation of 3,1-benzoxazin-2-ones as HIV reverse transcriptase inhibitors
 INVENTOR(S): Christ, David Donald; Markwalder, Jay Andrew; Fortunak, Joseph Marian; Ko, Soo Sung; Mutlib, Abdul Ezaz; Parsons, Rodney Lawrence, Jr.; Patel, Mona; Seitz, Steven Paul
 PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Co., USA
 SOURCE: PCT Int. Appl., 213 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9814436	A1	19980409	WO 1997-US17540	19971001
W: AU, BA, CA, CU, JP, LC, MX, NZ				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9708759	A	19990330	ZA 1997-8759	19970930
CA 2268953	A1	19980409	CA 1997-2268953	19971001
AU 9748027	A	19980424	AU 1997-48027	19971001
EP 929533	A1	19990721	EP 1997-910726	19971001
EP 929533	B1	20030903		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2001505873	T	20010508	JP 1998-516775	19971001
AT 248826	T	20030915	AT 1997-910726	19971001
EP 1359147	A1	20031105	EP 2003-12262	19971001
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
ES 2203790	T3	20040416	ES 1997-910726	19971001
PRIORITY APPLN. INFO.:				
			US 1996-725294	19961002
			US 1997-846578	19970430
			EP 1997-910726	19971001
			WO 1997-US17540	19971001

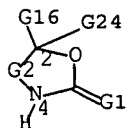
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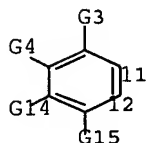
AB Title compds. [I; A = O or S; R1 = CF3, (cyclo)alkyl, alkenyl, etc.; R2 = QCHR7R8, QCHR7C.tplbond.R8, CH:CR7R8, etc.; Q = O, S, NH; R7 = H or alkyl; R8 = H, (cyclo)alkyl, Ph, heteroaryl, etc.; W = N or CR3; R3 = H, halo, alkyl, alkoxy; X = N or CR4; R4 = H, halo, alkyl, alkoxy, etc.; Y = N or CR5; R5 = H or halo; R4R5 = OCH2O or CH:CHCH:CH; Z = N or CR6 = H, halo, OH, alkoxy, etc.; ≤2 of W-Z = N] were prepared as HIV reverse transcriptase inhibitors (no data). Thus, 4,3-Cl(MeO)C6H3NHCOCMe3 (preparation given) was C-acylated by CF3CO2Et and the product converted in 3 steps to 3,5-Cl(Me3CMe2SiO)C6H3COCF3

which was treated with BuLi/HC.tplbond.C(CH₂)₃Cl and the product cyclocondensed with COCl₂ to give I [A = O, R₁ = CF₃, R₂ = cyclopropylethynyl, W = Y = CH, X = CCl, Z = C(OH)].

MSTR 1



G1 = O
G2 = 11-2 12-4



G4 = carbocycle <containing 6 C, aromatic,
bonds all normalized, 6-membered monocyclic ring>
(opt. substd. by (1-2) G13)
G13 = F
G16 = alkyl <containing 1-4 C>
G19 = carbon chain <0 or more double bonds,
0 or more triple bonds>
G24 = 161

181⁹-G17

Derivative:	or pharmaceutically acceptable salts
Patent location:	claim 1
Note:	substitution is restricted
Note:	also incorporates structure II in claim 6
Stereochemistry:	or stereoisomers

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 16 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No.	(AN): 2025595857 CHEMCATS
Catalog Name	(CO): Milestone PharmTech Product List
Publication Date	(PD): 27 Mar 2007
Order Number	(ON): 5B-0006
Chemical Name	(CN): 5-(4,4-dimethyl-2-oxo-2,4-dihydro-1H-benzo[d][1,3]oxazin-6-yl)-2-fluorobenzonitrile

INVENTOR SEARCH

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FILE LAST UPDATED: 11 Sep 2007 (20070911/ED)

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<http://www.cas.org/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

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L10          STR
L13          78 SEA FILE=REGISTRY SSS FUL L10
L15          7953 SEA FILE=CAPLUS ABB=ON  ZHANG P?/AU
L16          40 SEA FILE=CAPLUS ABB=ON  TEREFEENKO E?/AU
L17          72 SEA FILE=CAPLUS ABB=ON  FENSOME A?/AU
L18          634 SEA FILE=CAPLUS ABB=ON  WROBEL J?/AU
L19          406 SEA FILE=CAPLUS ABB=ON  FLETCHER H?/AU
L20          245 SEA FILE=CAPLUS ABB=ON  ZHI L?/AU
L21          3830 SEA FILE=CAPLUS ABB=ON  JONES T?/AU
L22          3382 SEA FILE=CAPLUS ABB=ON  EDWARDS J?/AU
L23          55 SEA FILE=CAPLUS ABB=ON  TEGLEY C?/AU
L24          13 SEA FILE=CAPLUS ABB=ON  L13
L25          9 SEA FILE=CAPLUS ABB=ON  (L15 OR L16 OR L17 OR L18 OR L19 OR
          L20 OR L21 OR L22 OR L23 OR L1) AND L24

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L25 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:77267 CAPLUS Full-text

DOCUMENT NUMBER: 144:171000

TITLE: Preparation of benzoxazinones and benzoxazinthiones as mineralocorticoid receptor modulators

INVENTOR(S): Higuchi, Robert I.; Zhi, Lin; Adams, Mark E.; Liu, Yan; Karanewsky, Donald S.

PATENT ASSIGNEE(S): Ligand Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 97 pp.

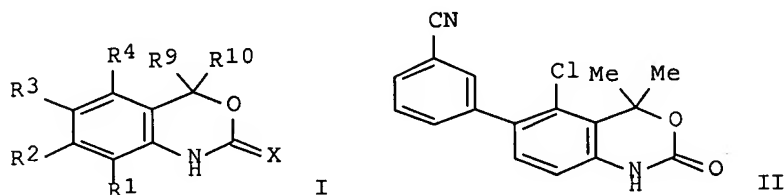
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006010142	A2	20060126	WO 2005-US24748	20050712
WO 2006010142	A3	20070104		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2007197520	A1	20070823	US 2007-622983	20070112
PRIORITY APPLN. INFO.:			US 2004-587947P	P 20040714
			WO 2005-US24748	A1 20050712
OTHER SOURCE(S):		MARPAT 144:171000		
GI				

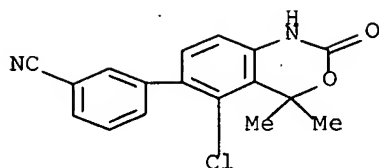


AB Title compds. I [R1 and R2 independently = F, Cl, CN. (un)substituted alkyl, etc.; R3 = (un)substituted aryl or heterocycle; R4 = H, halo, NO₂, etc.; R9 and R10 independently = H, (un)substituted alkyl, heteroalkyl, haloalkyl, etc.; X = O, S and NOR11 wherein R11 = H, (un)substituted alkyl, aryl, cycloalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as compds. that bind to mineralocorticoid receptors and/or modulate activity of mineralocorticoid receptors, and to methods for using such compds. Thus, e.g., II was prepared by coupling of 6-bromo-5-chloro-1,4-dihydro-4,4-dimethyl-2H-3,1-benzoxazin-2-one (preparation given) with 3-cyanophenylboronic acid. I were subjected to mineralocorticoid binding assays, e.g., II was determined to bind with a K_i value of 98.

IT 874472-53-4P 874472-64-7P 874472-76-1P
874472-78-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoxazinones and benzoxazinethiones as mineralocorticoid receptor modulators)

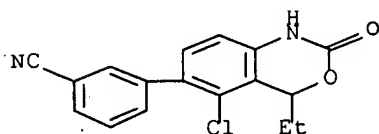
RN 874472-53-4 CAPLUS

CN Benzonitrile, 3-(5-chloro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



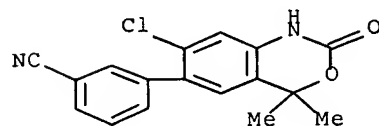
RN 874472-64-7 CAPLUS

CN Benzonitrile, 3-(5-chloro-4-ethyl-1,4-dihydro-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



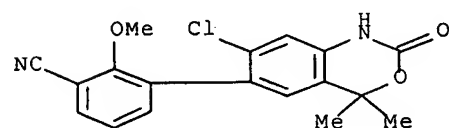
RN 874472-76-1 CAPLUS

CN Benzonitrile, 3-(7-chloro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



RN 874472-78-3 CAPLUS

CN Benzonitrile, 3-(7-chloro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-methoxy- (9CI) (CA INDEX NAME)



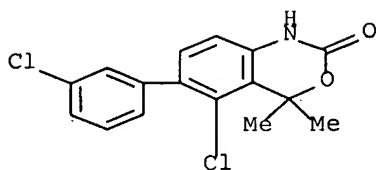
IT 874472-57-8P 874472-60-3P 874472-61-4P
874472-75-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazinones and benzoxazinthiones as mineralocorticoid receptor modulators)

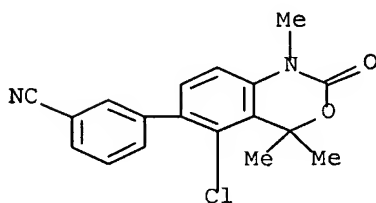
RN 874472-57-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 5-chloro-6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



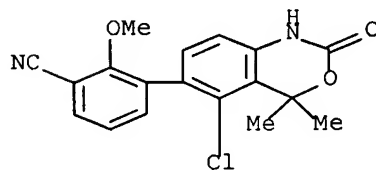
RN 874472-60-3 CAPLUS

CN Benzonitrile, 3-(5-chloro-1,4-dihydro-1,4,4-trimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



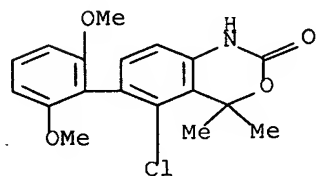
RN 874472-61-4 CAPLUS

CN Benzonitrile, 3-(5-chloro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-methoxy- (9CI) (CA INDEX NAME)



RN 874472-75-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 5-chloro-6-(2,6-dimethoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



L25 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:33235 CAPLUS Full-text

DOCUMENT NUMBER: 144:81462

TITLE: Progesterone receptor antagonists, contraceptive regimens, and kits

INVENTOR(S): Grubb, Gary Sondermann; Constantine, Ginger Dale;
Fensome, Andrew; McComas, Casey Cameron;
Melenski, Edward George; Marella, Michael Anthony;
Wrobel, Jay Edward

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: U.S. Pat. Appl. Publ., 22 pp.
CODEN: USXXCO

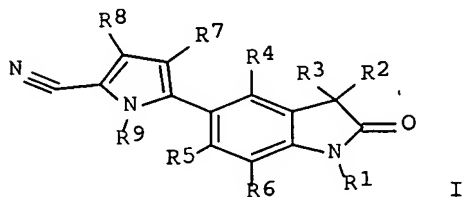
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006009509	A1	20060112	US 2005-175549	20050706
AU 2005271974	A1	20060216	AU 2005-271974	20050706
CA 2571198	A1	20060216	CA 2005-2571198	20050706
WO 2006017075	A1	20060216	WO 2005-US23798	20050706
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1773323	A1	20070418	EP 2005-771038	20050706
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CN 1980660	A	20070613	CN 2005-80022750	20050706
KR 2007039912	A	20070413	KR 2007-700184	20070104
IN 2007DN00304	A	20070817	IN 2007-DN304	20070111
NO 2007000377	A	20070207	NO 2007-377	20070119
PRIORITY APPLN. INFO.:			US 2004-585883P	P 20040707
			US 2005-676135P	P 20050429
			WO 2005-US23798	W 20050706
OTHER SOURCE(S):		MARPAT 144:81462		
GI				



AB A method of contraception is provided which involves delivery of 21 to 27 consecutive days of one or more progesterone receptor (PR) antagonists in the absence of a progestin, estrogen, or other steroidal compound, followed by 1 to 7 days without any active agent. Also described is a pharmaceutically

useful kit to facilitate delivery of this regimen. Example PR antagonists include mifepristone, onapristone, lilopristone, asoprisinyl, CDB-2914, substituted 1,4-dihydrobenzo[d][1,3]oxazin-2-ones, and carbonitriles of general formula I (wherein: R1 is H, (un)substituted alkyl, cycloalkyl, C3-C6 alkenyl, or C3-C6 alkynyl; R2 and R3 = H, (un)substituted alkyl; or R2 and R3 together form a ring; R4 = H or halogen; R5 = H; R6 = H or halogen; R7 = H, alkyl, or halogen; R8 = H; R9 = H, (un)substituted alkyl or COORA, where RA is alkyl or substituted alkyl).

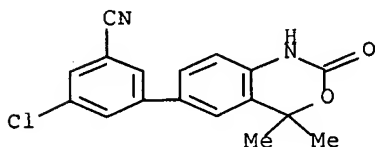
IT 304854-22-6P, 3-Chloro-5-(4,4-dimethyl-2-oxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)benzonitrile

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indole and benzoxazinone carbonitriles as progesterone receptor antagonists; progesterone receptor antagonists, contraceptive regimens, and kits)

RN 304854-22-6 CAPLUS

CN Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



L25 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:589387 CAPLUS Full-text

DOCUMENT NUMBER: 143:166013

TITLE: SAR studies of 6-aryl-1,3-dihydrobenzimidazol-2-ones as progesterone receptor antagonists

AUTHOR(S): Terefenko, Eugene A.; Kern, Jeffrey; Fensome, Andrew; Wrobel, Jay; Zhu, Yuan; Cohen, Jeffrey; Winneker, Richard; Zhang, Zhiming; Zhang, Puwen

CORPORATE SOURCE: Chemical and Screening Sciences, Wyeth Research, Collegeville, PA, 19426, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(15), 3600-3603

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:166013

AB We have previously reported that the aryl substituted benzimidazolones, benzoxazinones, and oxindoles (e.g., 1-3) are progesterone receptor (PR) antagonists and have recently disclosed that the nature of 5- and 6-aryl moieties played a critical role in PR functional activity in the oxindole and benzoxazinone templates. For example, replacing the Ph group of PR antagonists 2 and 3 with a 5'-cyanopyrrol-2'-yl moiety switched their functional activity to PR agonist activity (2a and 3a). These findings prompted us to examine if there is a similar effect of the 6-aryl moieties on the PR functional activity for the benzimidazolone template. Numerous analogs, such as 5, showed potent PR antagonist activity with about a 10-fold increase in potency as compared to those reported earlier in the same series. More interestingly, pyrrole-containing benzimidazolones 24-27 remained as PR

antagonists in contrast to the PR agonist activity switch for oxindole and benzoxazinone scaffolds when a 5'-cyanopyrrol-2'-yl group was installed as a pendant aryl group.

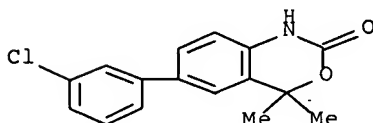
IT 304853-28-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(SAR studies of 6-aryl-1,3-dihydrobenzimidazol-2-ones as progesterone receptor antagonists)

RN 304853-28-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:303287 CAPLUS Full-text

DOCUMENT NUMBER: 141:54271

TITLE: Novel pyrrole-containing progesterone receptor modulators

AUTHOR(S): Collins, Mark A.; Hudak, Valerie; Bender, Reinhold; Fensome, Andrew; Zhang, Puwen; Miller, Lori; Winneker, Richard C.; Zhang, Zhiming; Zhu, Yuan; Cohen, Jeffrey; Unwalla, Raymond J.; Wrobel, Jay

CORPORATE SOURCE: Chemical and Screening Sciences, Wyeth Research, Collegeville, PA, 19426, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2185-2189

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:54271

AB A series of 1,4-dihydro-2H-[d][3,1]-benzoxazin-2-one and 1,3-dihydro-[3H]-indol-2-one containing 6- or 5-, resp., appended substituted pyrrole moieties were synthesized and evaluated for their ability to modulate the activity of the progesterone receptor (PR). Key structural changes to the pyrrole moieties of these mols. were shown to have a predictive influence as to whether the compds. behaved as PR agonists or antagonists. Compds. with the 5'-cyano-2'-pyrrole moiety were shown to be potent PR agonists (EC₅₀'s of 1.1, 1.8, and 2.8 nM, resp.). Compds. with the 5'-nitro-2'-pyrrole moiety were shown to be PR antagonists (IC₅₀'s of 180 and 36 nM, resp.).

IT 304854-16-8

RL: PAC (Pharmacological activity); BIOL (Biological study) (preparation of pyrrole-containing progesterone receptor modulators)

RN 304854-16-8 CAPLUS

CN 2-Furancarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

AB A method of contraception comprises administration to a female of a progestational agent in a first phase and in a second phase administration of [I; R1, R2 = H, (un)substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, aryl, heterocyclyl, amino derivative; R1R2 = atoms to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, C3-6 alkenyl, alkynyl, COR6; R6 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, alkynyl, C1-6 alkoxy, amino, C1-6 aminoalkyl; R5 = trisubstituted benzene ring, 5-6 membered ring with 1, 2, or 3 O, S, SO, SO2, NR7 and containing 1-2 H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, NR9COR8; R7 = H, C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl]. Thus, 6-(3-chlorophenyl)-4,4-dimethyl-1,4-dihydrobenzo[d][1,3]-oxazin-2-one was prepared from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. I demonstrated IC50's of 2.7-68 nM in a hPR decidualization assay.

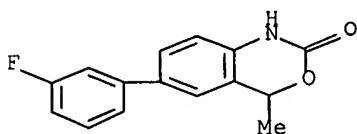
IT 304853-93-8P, 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4-methyl-

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

RN 304853-93-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4-methyl- (9CI)
(CA INDEX NAME)



IT 304853-28-9P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl- 304853-29-0P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 304853-30-3P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- 304853-36-9P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- 304854-07-7P, Benzonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- 304854-09-9P, 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-10-2P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-methylphenyl)-1,4-dihydro-4,4-dimethyl- 304854-11-3P, 2H-3,1-Benzoxazin-2-one, 6-[3-bromo-5-(trifluoromethoxy)phenyl]-1,4-dihydro-4,4-dimethyl- 304854-12-4P, Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-5-fluoro- 304854-13-5P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-methyl- 304854-14-6P, 2H-3,1-Benzoxazin-2-one, 6-(3,5-dichlorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-15-7P, 1,3-Benzenedicarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- 304854-16-8P, 2-Furancarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- 304854-21-5P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(2-propenyl)- 304854-22-6P, Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-

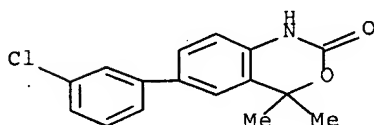
304854-23-7P, 2H-3,1-Benzoxazin-2-one, 6-(3,5-difluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-24-8P, 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- 304854-25-9P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-methoxy- 304854-26-0P, 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-27-1P, 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(trifluoromethyl)phenyl]-1,4-dihydro-4,4-dimethyl- 304854-28-2P, 2H-3,1-Benzoxazin-2-one, 6-(2-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-29-3P, 2H-3,1-Benzoxazin-2-one, 6-(3,4-difluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-30-6P, 2H-3,1-Benzoxazin-2-one, 6-(4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-31-7P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro- 304854-32-8P, 2H-3,1-Benzoxazin-2-one, 6-(2,3-difluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-33-9P, Benzonitrile, 3-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- 304854-35-1P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4,4-diethyl-1,4-dihydro- 304854-36-2P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-6-(3-methoxyphenyl)-4,4-dimethyl- 304854-37-3P, 2H-3,1-Benzoxazin-2-one, 6-(2-chlorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-41-9P, Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- 304854-42-0P, Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)- 304854-45-3P, 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-47-5P, 2-Furancarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- 304854-49-7P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-4,4-dimethyl- 305799-74-0P, 2H-3,1-Benzoxazin-2-one, 6-(4-chlorophenyl)-1,4-dihydro-4,4-dimethyl- 305799-76-2P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl- 305799-78-4P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethyl-1,4-dihydro- 305799-83-1P, Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2-one, 6-(3-chlorophenyl)-1,2-dihydro- 305799-85-3P, Spiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-one, 6-(3-chlorophenyl)- 305799-87-5P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(1-propynyl)- 305799-88-6P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethynyl-1,4-dihydro-4-methyl- 305799-97-7P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-di-1-propynyl- 305799-98-8P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-1,4,4-trimethyl- 305800-11-7P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-(trifluoromethoxy)- 305800-18-4P, 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-8-fluoro-1,4-dihydro-4,4-dimethyl- 305800-22-0P, 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-nitrophenyl)-1,4-dihydro-4,4-dimethyl- 305800-46-8P, Benzonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- 305800-48-0P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- 305800-50-4P, Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one, 6-(3-methoxyphenyl)- 305800-51-5P, 2H-3,1-Benzoxazin-2-one, 8-bromo-6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 305800-52-6P, Benzonitrile, 5-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- 305800-53-7P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-1,4,4-trimethyl- 305800-55-9P, Benzonitrile, 3-(1,4-dihydro-8-methoxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- 305800-56-0P, Benzonitrile, 3-(1,4-dihydro-8-hydroxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- 305800-57-1P, Benzonitrile, 3-(1-ethyl-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- 305800-59-3P,

Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- 305800-62-8P, Benzeneacetonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- 305800-64-0P, Acetamide, N-[4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluorophenyl]- 305800-65-1P, 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-4-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- 305800-71-9P, 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- 305800-72-0P, 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-, 2-oxime 305839-71-8P, 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(2-thienyl)phenyl]-1,4-dihydro-4,4-dimethyl- 305839-75-2P, Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro- 305839-76-3P, 2H-3,1-Benzoxazin-2-one, 6-[5-(diethoxymethyl)-2-furanyl]-1,4-dihydro-4,4-dimethyl-
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

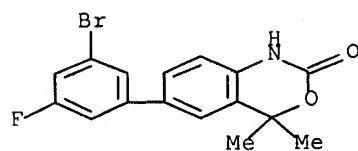
RN 304853-28-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



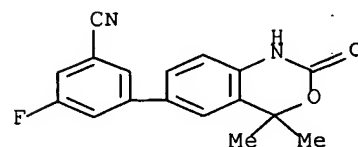
RN 304853-29-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



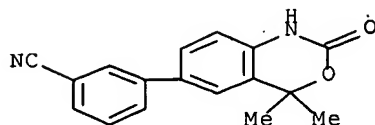
RN 304853-30-3 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



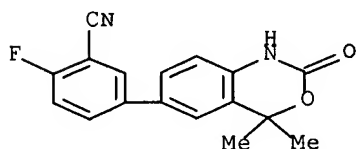
RN 304853-36-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
(9CI) (CA INDEX NAME)



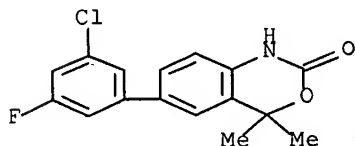
RN 304854-07-7 CAPLUS

CN Benzonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



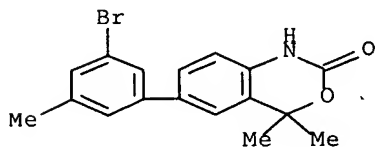
RN 304854-09-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



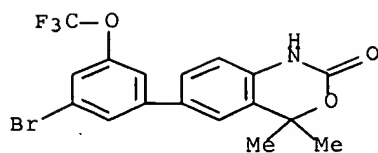
RN 304854-10-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-methylphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



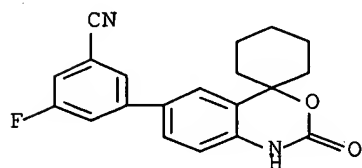
RN 304854-11-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-bromo-5-(trifluoromethoxy)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



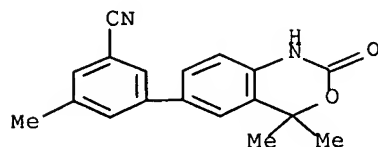
RN 304854-12-4 CAPLUS

CN Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



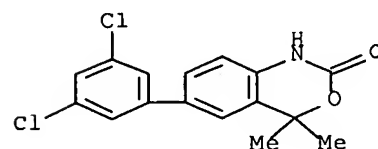
RN 304854-13-5 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-methyl- (9CI) (CA INDEX NAME)



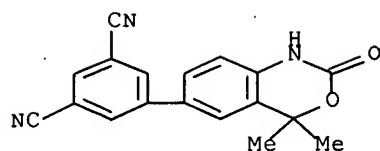
RN 304854-14-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3,5-dichlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



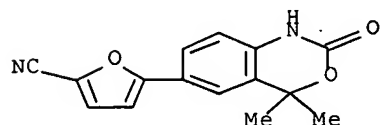
RN 304854-15-7 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



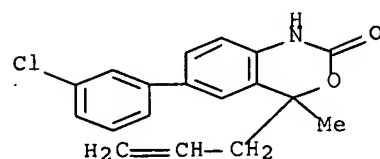
RN 304854-16-8 CAPLUS

CN 2-Furancarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



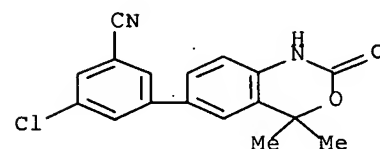
RN 304854-21-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(2-propenyl)- (9CI) (CA INDEX NAME)



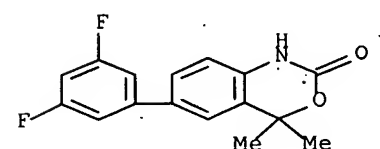
RN 304854-22-6 CAPLUS

CN Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



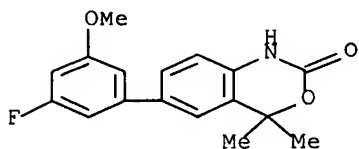
RN 304854-23-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3,5-difluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



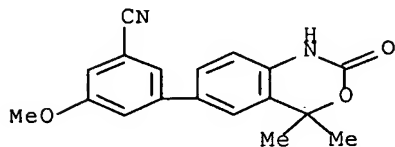
RN 304854-24-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



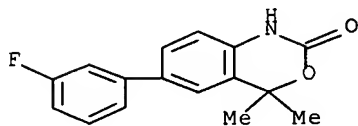
RN 304854-25-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-methoxy- (9CI) (CA INDEX NAME)



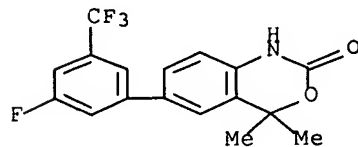
RN 304854-26-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



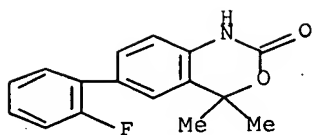
RN 304854-27-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(trifluoromethyl)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



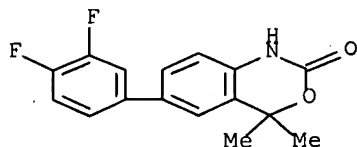
RN 304854-28-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



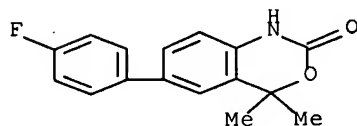
RN 304854-29-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3,4-difluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



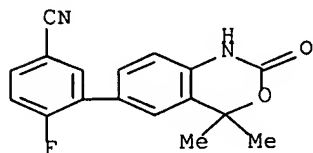
RN 304854-30-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(4-fluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



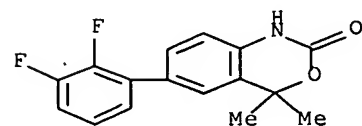
RN 304854-31-7 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro- (9CI) (CA INDEX NAME)



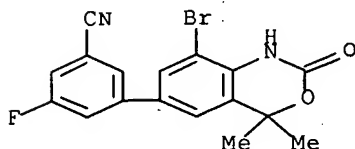
RN 304854-32-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2,3-difluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



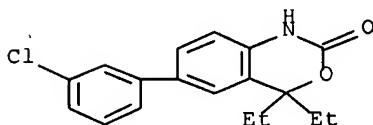
RN 304854-33-9 CAPLUS

CN Benzonitrile, 3-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



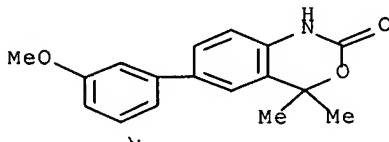
RN 304854-35-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4,4-diethyl-1,4-dihydro- (9CI) (CA INDEX NAME)



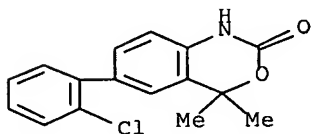
RN 304854-36-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-6-(3-methoxyphenyl)-4,4-dimethyl- (9CI) (CA INDEX NAME)



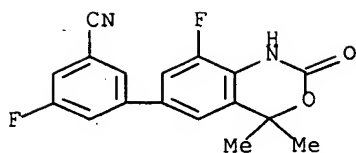
RN 304854-37-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2-chlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



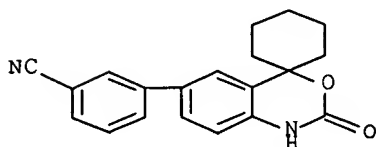
RN 304854-41-9 CAPLUS

CN Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



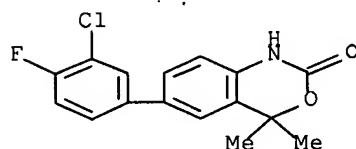
RN 304854-42-0 CAPLUS

CN Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)- (9CI) (CA INDEX NAME)



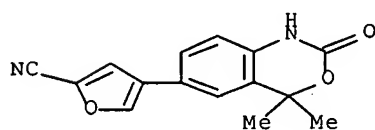
RN 304854-45-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



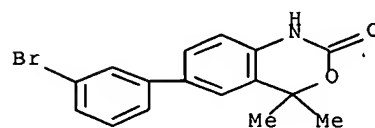
RN 304854-47-5 CAPLUS

CN 2-Furancarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

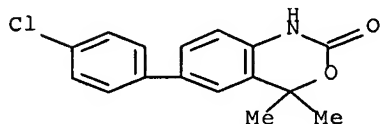


RN 304854-49-7 CAPLUS

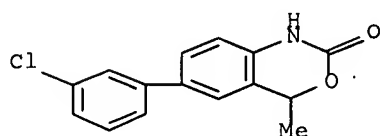
CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



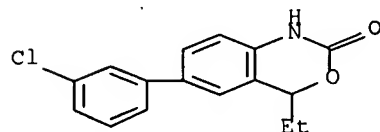
RN 305799-74-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(4-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)

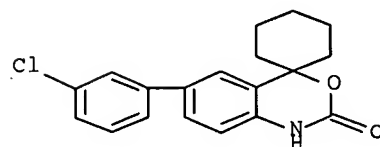
RN 305799-76-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl- (9CI)
(CA INDEX NAME)

RN 305799-78-4 CAPLUS

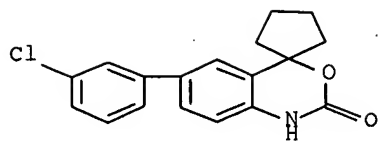
CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethyl-1,4-dihydro- (9CI)
(CA INDEX NAME)

RN 305799-83-1 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one, 6-(3-chlorophenyl)-
(9CI) (CA INDEX NAME)

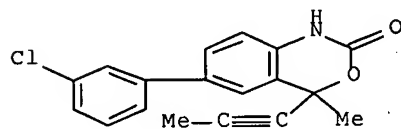
RN 305799-85-3 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-one, 6-(3-chlorophenyl)-
(9CI) (CA INDEX NAME)



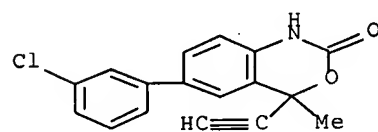
RN 305799-87-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(1-propynyl)- (9CI) (CA INDEX NAME)



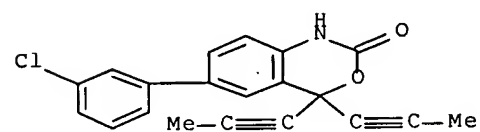
RN 305799-88-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethynyl-1,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)



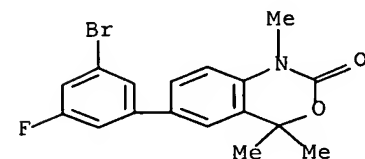
RN 305799-97-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-di-1-propynyl- (9CI) (CA INDEX NAME)



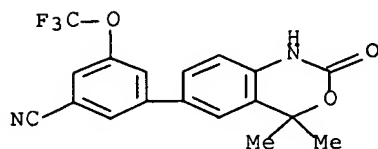
RN 305799-98-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-1,4,4-trimethyl- (9CI) (CA INDEX NAME)



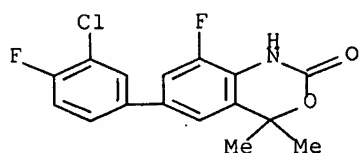
RN 305800-11-7 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



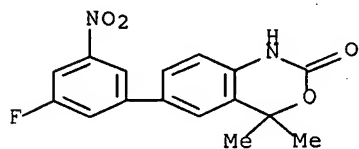
RN 305800-18-4 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-8-fluoro-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



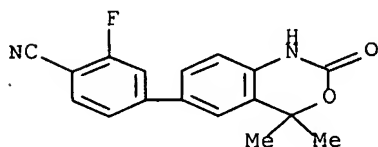
RN 305800-22-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-nitrophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



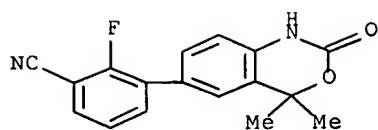
RN 305800-46-8 CAPLUS

CN Benzonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



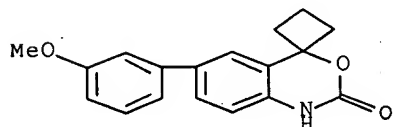
RN 305800-48-0 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



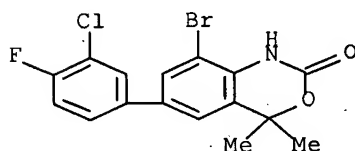
RN 305800-50-4 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one, 6-(3-methoxyphenyl)-
(9CI) (CA INDEX NAME)



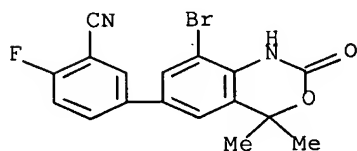
RN 305800-51-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 8-bromo-6-(3-chloro-4-fluorophenyl)-1,4-dihydro-
4,4-dimethyl- (9CI) (CA INDEX NAME)



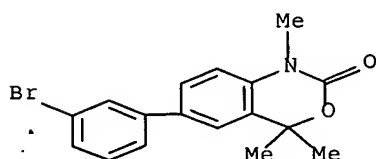
RN 305800-52-6 CAPLUS

CN Benzonitrile, 5-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-
6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



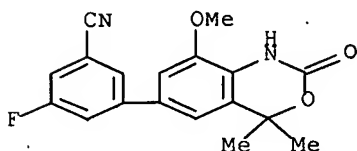
RN 305800-53-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-1,4,4-trimethyl-
(9CI) (CA INDEX NAME)



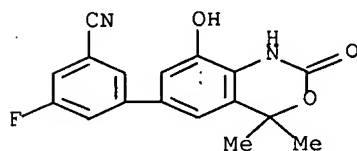
RN 305800-55-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-8-methoxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



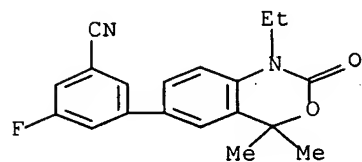
RN 305800-56-0 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-8-hydroxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



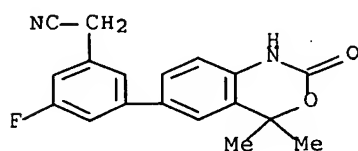
RN 305800-57-1 CAPLUS

CN Benzonitrile, 3-(1-ethyl-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



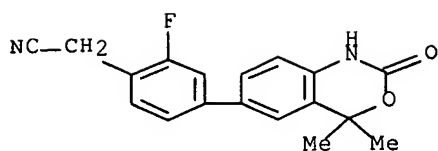
RN 305800-59-3 CAPLUS

CN Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



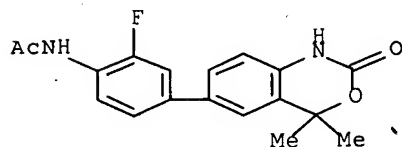
RN 305800-62-8 CAPLUS

CN Benzeneacetonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



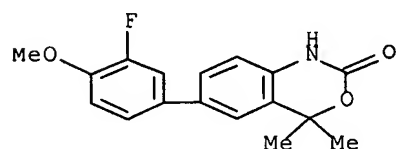
RN 305800-64-0 CAPLUS

CN Acetamide, N-[4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluorophenyl]- (9CI) (CA INDEX NAME)



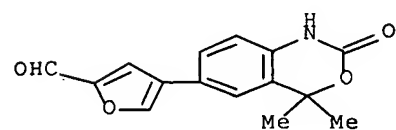
RN 305800-65-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-4-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



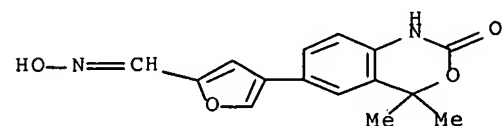
RN 305800-71-9 CAPLUS

CN 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



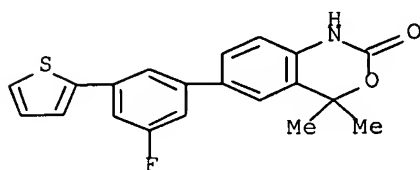
RN 305800-72-0 CAPLUS

CN 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-, 2-oxime (9CI) (CA INDEX NAME)



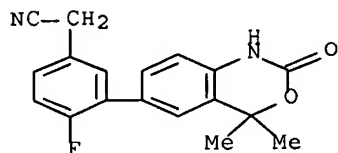
RN 305839-71-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(2-thienyl)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



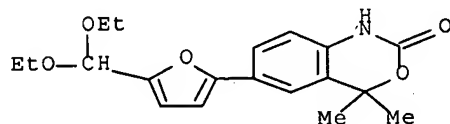
RN 305839-75-2 CAPLUS

CN Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro- (9CI) (CA INDEX NAME)



RN 305839-76-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[5-(diethoxymethyl)-2-furanyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:650988 CAPLUS Full-text

DOCUMENT NUMBER: 137:319962

TITLE: 6-Aryl-1,4-dihydro-benzo[d][1,3]oxazin-2-ones: A Novel Class of Potent, Selective, and Orally Active Nonsteroidal Progesterone Receptor Antagonists

AUTHOR(S): Zhang, Puwen; Terefenko, Eugene A.
; Fensome, Andrew; Wrobel, Jay;
Winneker, Richard; Lundeen, Scott; Marschke, Keith B.;
Zhang, Zhiming

CORPORATE SOURCE: Women's Health Research Institute, Chemical Sciences,
Wyeth Research, Collegeville, PA, 19426, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(20),
4379-4382

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:319962

AB Novel 6-aryl-1,4-dihydro-benzo[d][1,3]oxazin-2-ones were synthesized and tested as progesterone receptor (PR) antagonists. These compds. were potent and showed good selectivity for PR over other steroid receptors such as the glucocorticoid and androgen receptors (e.g., greater than 80-fold selectivity at PR). Numerous 6-aryl benzoxazinones were active orally in the uterine decidualization and component C3 assays in the rats.

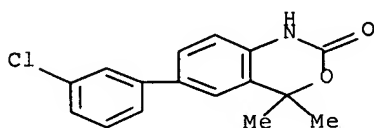
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304854-36-2P 304854-37-3P 304854-41-9P
304854-45-3P 304854-47-5P 305799-74-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and structure activity relationship of benzoxazinones as orally active nonsteroidal progesterone receptor antagonists)

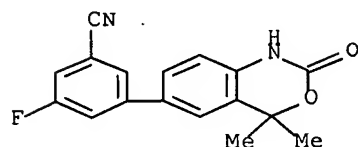
RN 304853-28-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



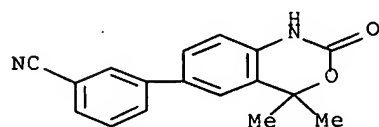
RN 304853-30-3 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



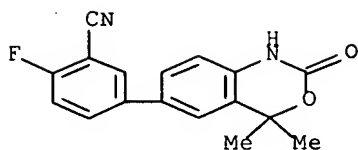
RN 304853-36-9 CAPLUS

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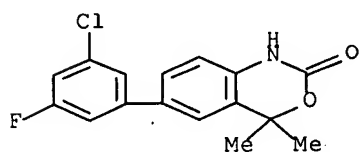
RN 304854-07-7 CAPLUS

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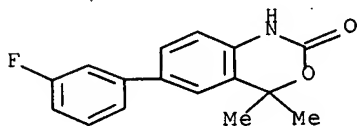
RN 304854-09-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



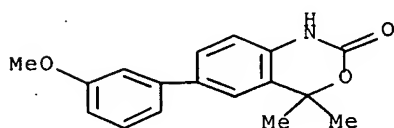
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CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



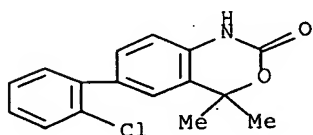
RN 304854-36-2 CAPLUS

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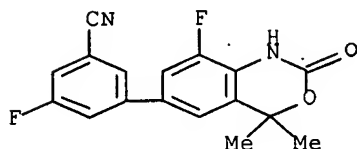
RN 304854-37-3 CAPLUS

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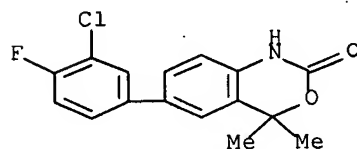
RN 304854-41-9 CAPLUS

CN Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



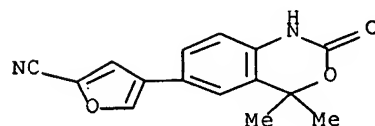
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CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



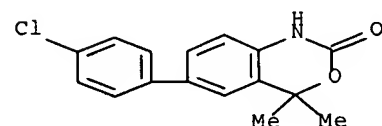
RN 304854-47-5 CAPLUS

CN 2-Furancarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



RN 305799-74-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(4-chlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

30

THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:790489 CAPLUS Full-text

DOCUMENT NUMBER: 133:350229

TITLE: Novel cyclocarbamate derivatives as progesterone receptor modulators

INVENTOR(S): Zhang, Puwen; Terefenko, Eugene A.
; Fletcher, Horace, III; Fensome,
Andrew; Wrobel, Jay E.; Zhi,
Lin; Jones, Todd K.; Marschke, Keith
B.; Tegley, Christopher M.

PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand
Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2

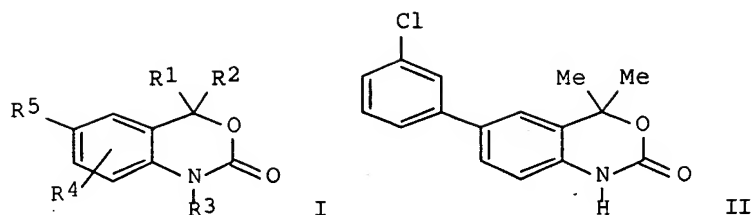
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066571	A1	20001109	WO 2000-US11822	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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BR 2000010213	A	20020219	BR 2000-10213	20000501
TR 200103286	T2	20020722	TR 2001-3286	20000501
HU 200201609	A2	20020828	HU 2002-1609	20000501
JP 2002543193	T	20021217	JP 2000-615601	20000501
AU 766428	B2	20031016	AU 2000-46886	20000501
NZ 515355	A	20040227	NZ 2000-515355	20000501
SG 114650	A1	20050928	SG 2004-80	20000501
US 2002049204	A1	20020425	US 2001-948309	20010906
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ZA 2001007630	A	20020514	ZA 2001-7630	20010917
IN 2001MN01295	A	20050318	IN 2001-MN1295	20011018
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NO 321361	B1	20060502		
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US 2003216388	A1	20031120	US 2003-386799	20030312
US 6713478	B2	20040330		
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PRIORITY APPLN. INFO.:			US 1999-183012P	P 19990504
			US 2000-552633	A1 20000419
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			US 2003-386799	A1 20030312
OTHER SOURCE(S):		MARPAT 133:350229		
GI				



AB This invention discloses novel aryl fused cyclocarbamate derivs. I (R1 or R2 = H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, (un)substituted C3-8 cycloalkyl, (un)substituted aryl, (un)substituted heterocyclyl, amino derivative or R1 and R2 may be fused to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, (un)substituted C3-6 alkenyl, (un)substituted alkynyl, or COR6 {R6 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy, or (un)substituted C1-3 aminoalkyl}; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, (un)substituted alkynyl, (un)substituted C1-6 alkoxy, amino, or (un)substituted C1-6 aminoalkyl; R5 = trisubstituted benzene ring or a five- or six-membered ring with 1, 2, or 3 heteroatoms selected from O, S, SO, SO2 or NR7 and containing one or two independent substituents from the group including H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, or NR9COR8 {R7 = H or C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy or (un)substituted C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl}) or pharmaceutically acceptable salts thereof, as well as pharmaceutical compns. and methods using the compds. as antagonists of the progesterone receptor. Thus, cyclocarbamate II was prepared from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. Compds. of the invention demonstrated potency in the range of 0.01 nM to 5 μ M in the in vitro assays, and 0.001 to 300 mg/kg in the in vivo assays.

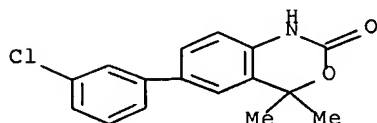
IT 304853-28-9P 304853-29-0P 304853-30-3P
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304854-49-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of benzoxazinone derivs. as progesterone receptor modulators)

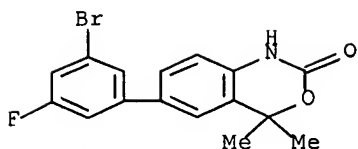
RN 304853-28-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



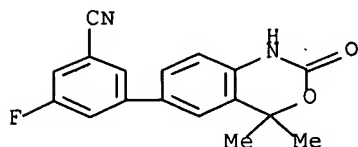
RN 304853-29-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



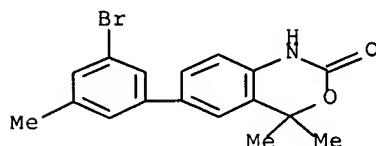
RN 304853-30-3 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



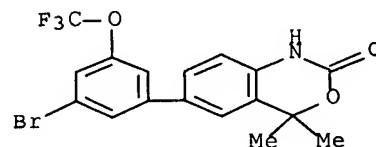
RN 304854-10-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-methylphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



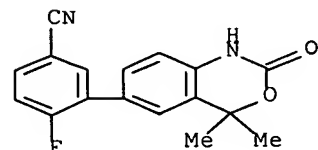
RN 304854-11-3 CAPLUS

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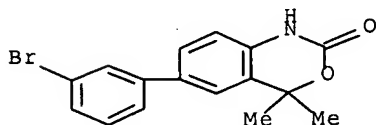


RN 304854-31-7 CAPLUS

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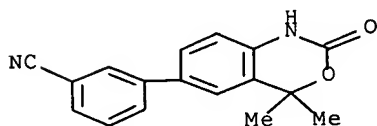
RN 304854-49-7 CAPLUS
 CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-4,4-dimethyl- (9CI)
 (CA INDEX NAME)



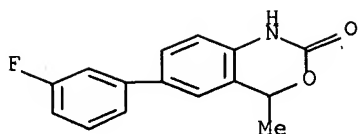
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 305839-76-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of benzoxazinone derivs. as progesterone receptor modulators)

RN 304853-36-9 CAPLUS
 CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

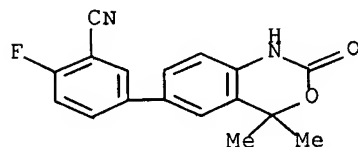


RN 304853-93-8 CAPLUS
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 (CA INDEX NAME)



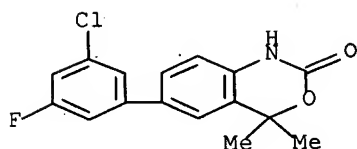
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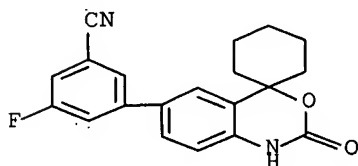
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CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



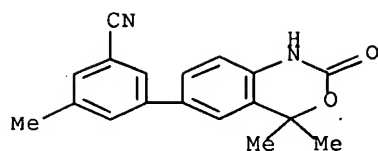
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CN Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



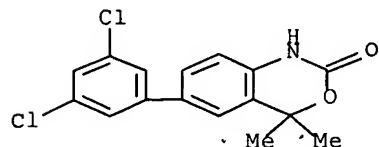
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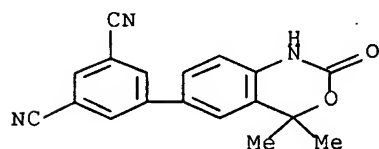
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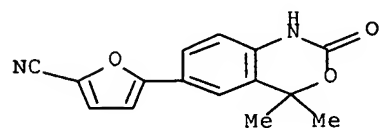
RN 304854-15-7 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



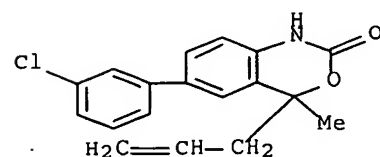
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CN 2-Furancarboxitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

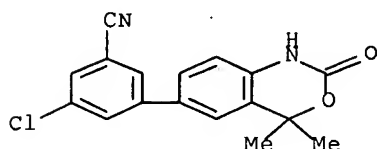


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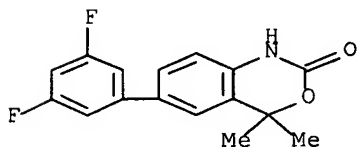
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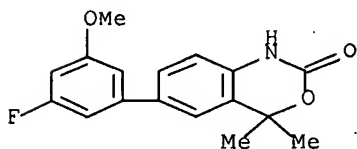
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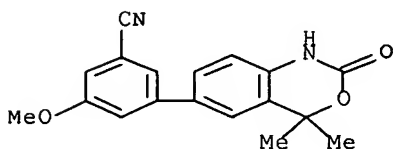
RN 304854-23-7 CAPLUS
 CN 2H-3,1-Benzoxazin-2-one, 6-(3,5-difluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



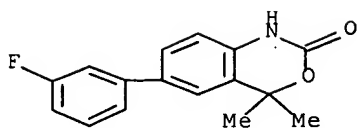
RN 304854-24-8 CAPLUS
 CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



RN 304854-25-9 CAPLUS
 CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-methoxy- (9CI) (CA INDEX NAME)

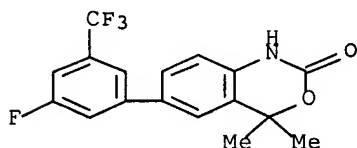


RN 304854-26-0 CAPLUS
 CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



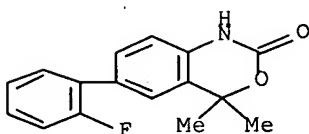
RN 304854-27-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(trifluoromethyl)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



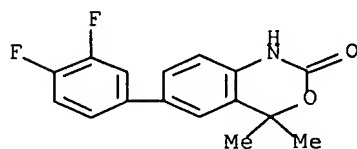
RN 304854-28-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



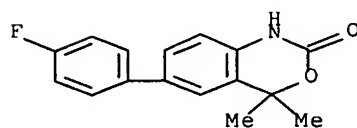
RN 304854-29-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3,4-difluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

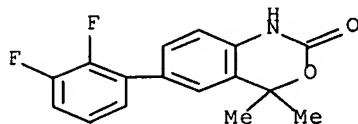


RN 304854-30-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

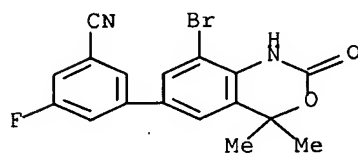


RN 304854-32-8 CAPLUS

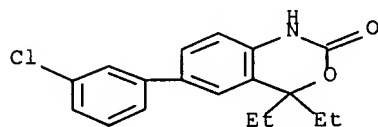
CN 2H-3,1-Benzoxazin-2-one, 6-(2,3-difluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)

RN 304854-33-9 CAPLUS

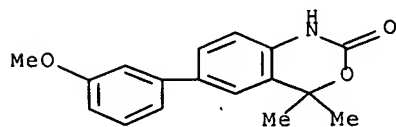
CN Benzonitrile, 3-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



RN 304854-35-1 CAPLUS

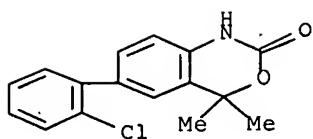
CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4,4-diethyl-1,4-dihydro- (9CI)
(CA INDEX NAME)

RN 304854-36-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-6-(3-methoxyphenyl)-4,4-dimethyl-
(9CI) (CA INDEX NAME)

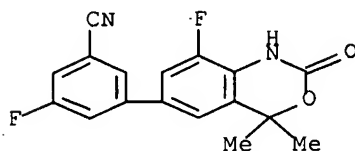
RN 304854-37-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



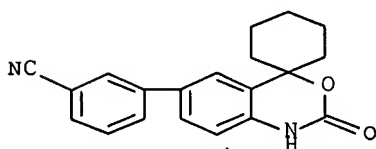
RN 304854-41-9 CAPLUS

CN Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



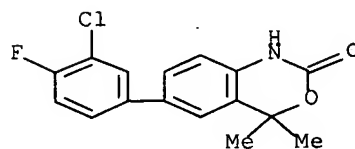
RN 304854-42-0 CAPLUS

CN Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)- (9CI) (CA INDEX NAME)



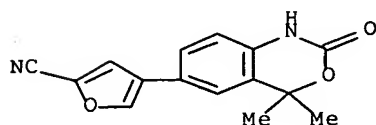
RN 304854-45-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

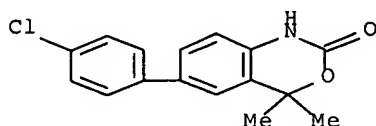


RN 304854-47-5 CAPLUS

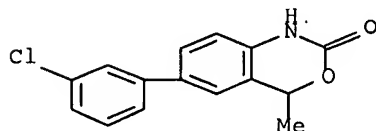
CN 2-Furancarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



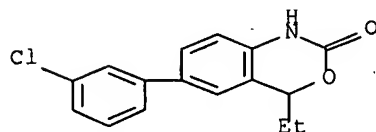
RN 305799-74-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(4-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)

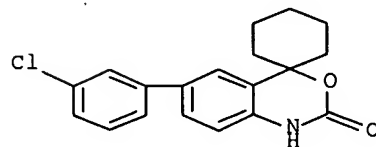
RN 305799-76-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl- (9CI)
(CA INDEX NAME)

RN 305799-78-4 CAPLUS

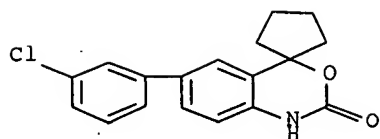
CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethyl-1,4-dihydro- (9CI)
(CA INDEX NAME)

RN 305799-83-1 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one, 6-(3-chlorophenyl)-
(9CI) (CA INDEX NAME)

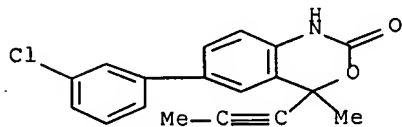
RN 305799-85-3 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-one, 6-(3-chlorophenyl)-
(9CI) (CA INDEX NAME)



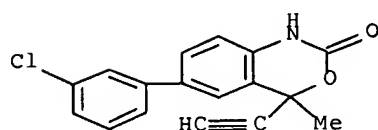
RN 305799-87-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(1-propynyl)- (9CI) (CA INDEX NAME)



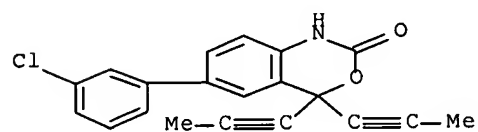
RN 305799-88-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethynyl-1,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)



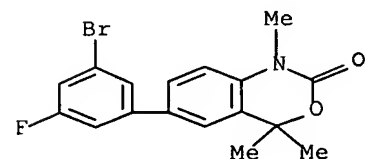
RN 305799-97-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-di-1-propynyl- (9CI) (CA INDEX NAME)



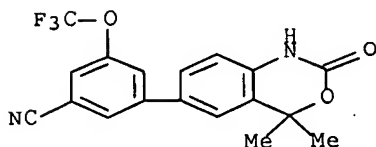
RN 305799-98-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-1,4,4-trimethyl- (9CI) (CA INDEX NAME)



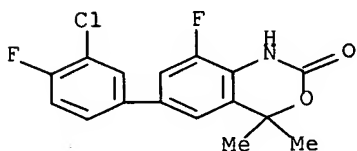
RN 305800-11-7 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



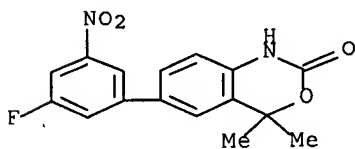
RN 305800-18-4 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-8-fluoro-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



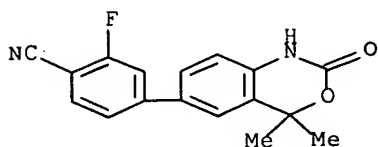
RN 305800-22-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-nitrophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



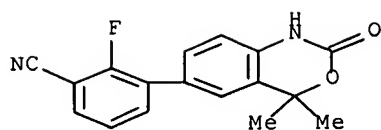
RN 305800-46-8 CAPLUS

CN Benzonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



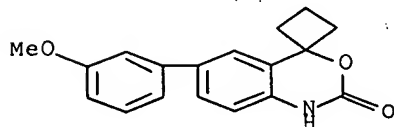
RN 305800-48-0 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



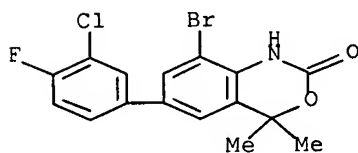
RN 305800-50-4 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one, 6-(3-methoxyphenyl)-(9CI) (CA INDEX NAME)



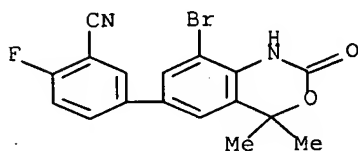
RN 305800-51-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 8-bromo-6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



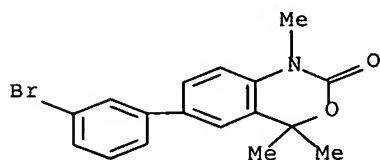
RN 305800-52-6 CAPLUS

CN Benzonitrile, 5-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



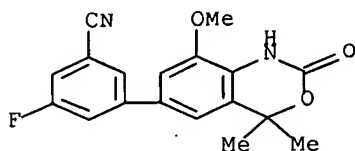
RN 305800-53-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-1,4,4-trimethyl-(9CI) (CA INDEX NAME)



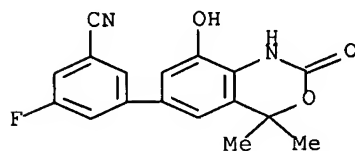
RN 305800-55-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-8-methoxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



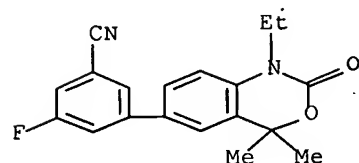
RN 305800-56-0 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-8-hydroxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



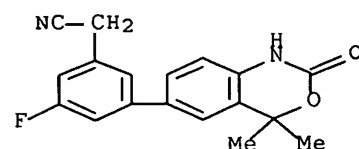
RN 305800-57-1 CAPLUS

CN Benzonitrile, 3-(1-ethyl-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



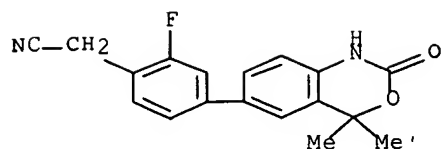
RN 305800-59-3 CAPLUS

CN Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



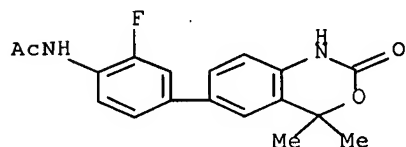
RN 305800-62-8 CAPLUS

CN Benzeneacetonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



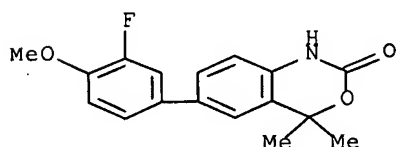
RN 305800-64-0 CAPLUS

CN Acetamide, N-[4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluorophenyl]- (9CI) (CA INDEX NAME)



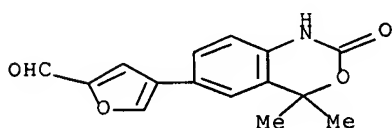
RN 305800-65-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-4-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



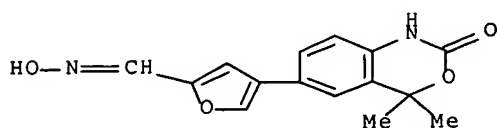
RN 305800-71-9 CAPLUS

CN 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



RN 305800-72-0 CAPLUS

CN 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-, 2-oxime (9CI) (CA INDEX NAME)



were prepared E.g., a multi-step synthesis of I [R1, R2 = Me; R3, R4 = H; R5 = 3-ClC6H4; Q1 = S] which showed EC50 of 0.65 nM against hPR in CV-1 cells, was given.

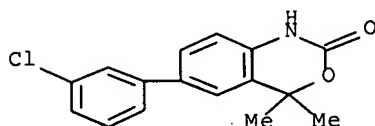
IT 304853-28-9P 304853-29-0P 304853-30-3P
304853-36-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of cyclothiocarbamate derivs. as progesterone receptor modulators)

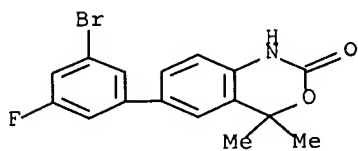
RN 304853-28-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



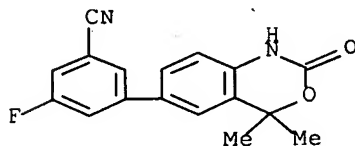
RN 304853-29-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



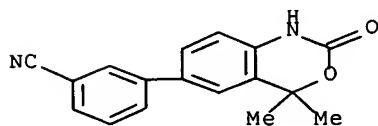
RN 304853-30-3 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



RN 304853-36-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
(9CI) (CA INDEX NAME)

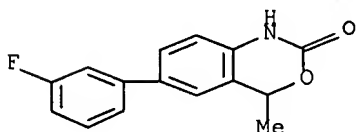


IT 304853-93-8P 304854-07-7P 304854-09-9P
 304854-10-2P 304854-11-3P 304854-12-4P
 304854-13-5P 304854-14-6P 304854-15-7P
 304854-16-8P 304854-21-5P 304854-22-6P
 304854-23-7P 304854-24-8P 304854-25-9P
 304854-26-0P 304854-27-1P 304854-28-2P
 304854-29-3P 304854-30-6P 304854-31-7P
 304854-32-8P 304854-33-9P 304854-35-1P
 304854-36-2P 304854-37-3P 304854-41-9P
 304854-42-0P 304854-45-3P 304854-47-5P
 304854-49-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of cyclothiocarbamate derivs. as progesterone receptor
 modulators)

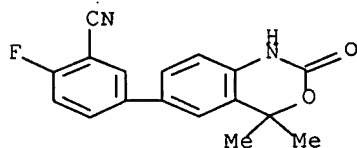
RN 304853-93-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4-methyl- (9CI)
 (CA INDEX NAME)



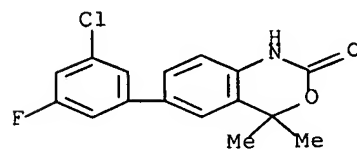
RN 304854-07-7 CAPLUS

CN Benzonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



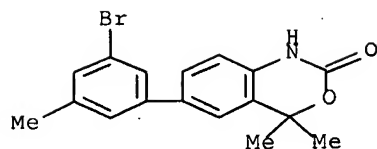
RN 304854-09-9 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



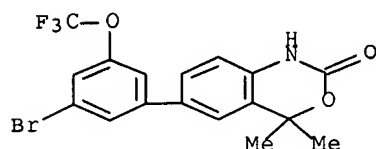
RN 304854-10-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-methylphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



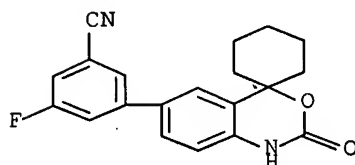
RN 304854-11-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-bromo-5-(trifluoromethoxy)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



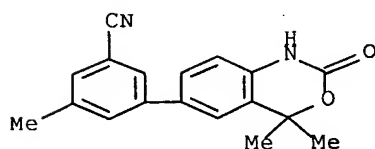
RN 304854-12-4 CAPLUS

CN Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



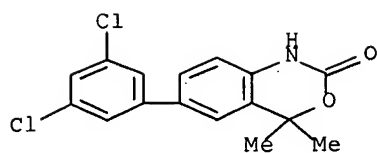
RN 304854-13-5 CAPLUS

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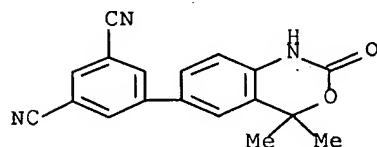
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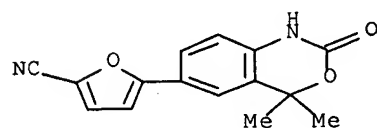
RN 304854-15-7 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



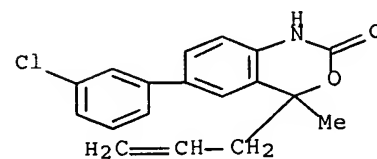
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CN 2-Furancarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



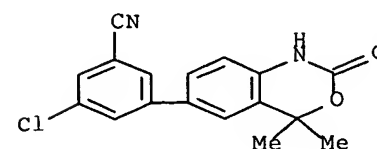
RN 304854-21-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(2-propenyl)- (9CI) (CA INDEX NAME)



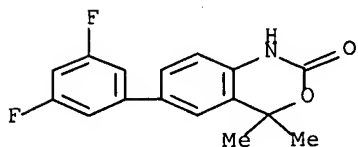
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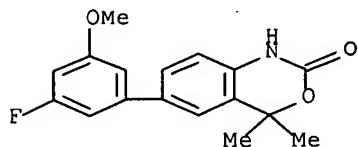
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CN 2H-3,1-Benzoxazin-2-one, 6-(3,5-difluorophenyl)-1,4-dihydro-4,4-dimethyl-
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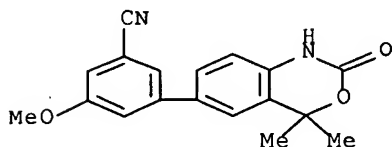
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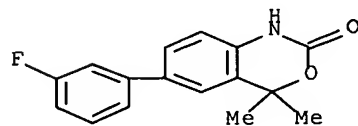
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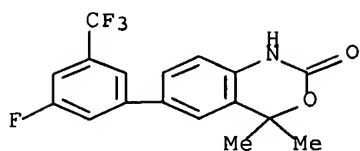
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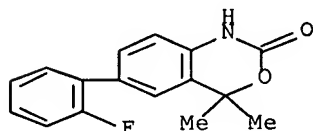
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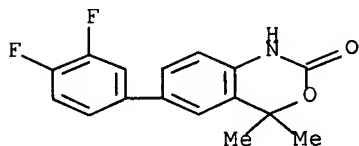
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CN 2H-3,1-Benzoxazin-2-one, 6-(2-fluorophenyl)-1,4-dihydro-4,4-dimethyl-
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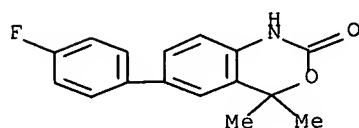
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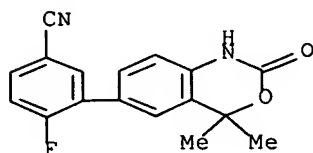
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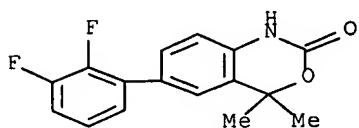


RN 304854-31-7 CAPLUS

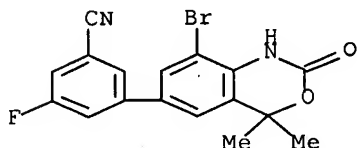
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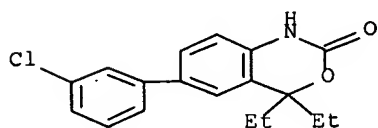
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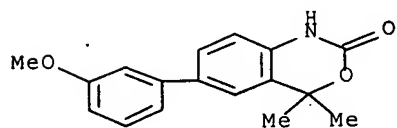
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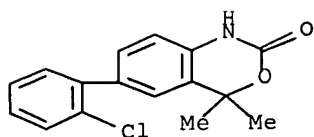
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 (CA INDEX NAME)



RN 304854-36-2 CAPLUS
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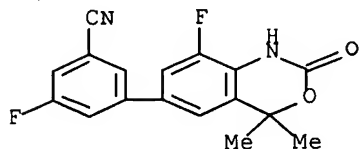


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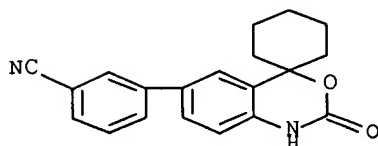
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CN Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



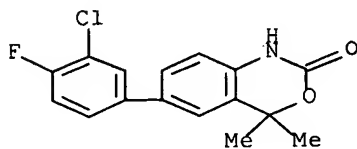
RN 304854-42-0 CAPLUS

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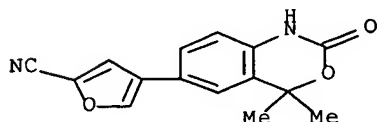
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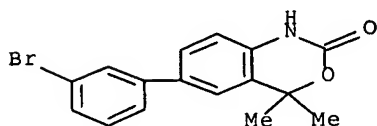


RN 304854-47-5 CAPLUS

CN 2-Furancarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



RN 304854-49-7 CAPLUS
 CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-4,4-dimethyl- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

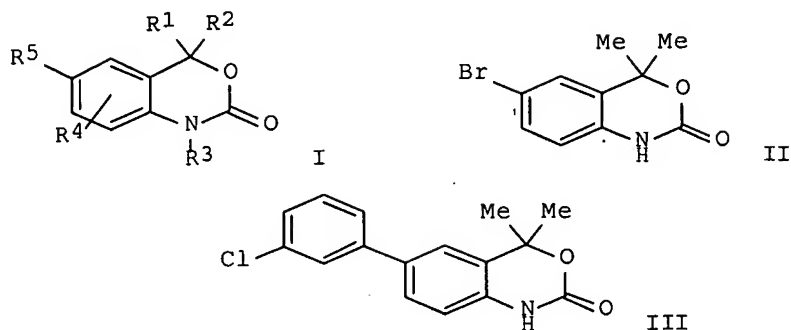
L25 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:790347 CAPLUS Full-text
 DOCUMENT NUMBER: 133:350205
 TITLE: Contraceptive compositions containing antiprogestinic
 and progestinic dihydro-2H-3,1-benzoxazin-2-ones
 INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd
 K.; Marschke, Keith B.; Tegley, Christopher
 M.
 PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand
 Pharmaceuticals, Inc.
 SOURCE: PCT Int. Appl., 146 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066164	A1	20001109	WO 2000-US11643	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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US 6498154	B1	20021224	US 2000-552357	20000419
CA 2372773	A1	20001109	CA 2000-2372773	20000501
EP 1173210	A1	20020123	EP 2000-928611	20000501
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JP 2002543155	T	20021217	JP 2000-615048	20000501
AT 275973	T	20041015	AT 2000-928611	20000501
TW 265032	B	20061101	TW 2000-89108477	20000725
MX 2001PA11311	A	20030714	MX 2001-PA11311	20011105
HK 1043736	A1	20050401	HK 2002-104868	20020628
PRIORITY APPLN. INFO.:			US 1999-304712	A 19990504
			US 2000-552357	A1 20000419
			US 1999-183042P	P 19990504
			US 2000-552350	A 20000419
			WO 2000-US11643	W 20000501

OTHER SOURCE(S):

MARPAT 133:350205

GI



AB The dihydrobenzoxazinones I [R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, acyl, acylamino; or R1R2 are fused to form spirocyclic or hetero-spirocyclic rings substituted by F, alkyl, alkoxy, alkylthio, F3C, HO, cyano, H2N, alkylamino; R3 = H, OH, NH2, C1-6 alkyl, C3-6 alkenyl, alkynyl, CORC; RC = H, C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, cyano, NO2, alkyl, alkynyl, alkoxy, alkoxy, amino, aminoalkyl; R5 = XYZC6H2, X = halo, cyano, alkyl, alkenyl, alkynyl, alkoxy, thioalkoxy, H2N, aminoalkyl, NO2, perfluoroalkyl, 5- or 6-membered heterocyclyl; Y, Z = H, halo, cyano, NO2, H2N, aminoalkyl, alkoxy, alkyl, thioalkoxy; or R5 = 5- or 6-membered heterocyclyl with O, S, SO, SO2 heteroatoms substituted by H, halo, cyano, NO2, H2N, alkyl, alkoxy, perfluoroacyl, perfluoroacylamino] and their pharmaceutically acceptable salts were prepared as antagonists of the progesterone receptor and were useful to induce contraception in mammals in cyclic combination therapies using an antiprogesterin and progesterin where the progesterin is administered in the alternating presence and absence of an antiprogesterin. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects of cyclic menstrual bleeding. Addnl. uses of the invention include stimulation of food intake. Thus, cyclocondensation of 2-(2-amino-5-bromophenyl)-2-propanol with carbonyldiimidazole gave the dimethylbenzoxazinone II which coupled with 3-chlorophenylboronic acid in DME/H2O containing (Ph3P)4Pd and Na2CO3 to give the (chlorophenyl)benzoxazinone III.

IT 304853-29-0P 304853-30-3P 304854-07-7P
304854-49-7P

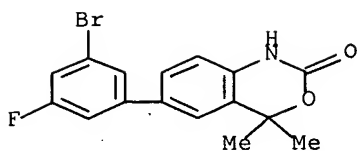
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(preparation of substituted dihydrobenzoxazinones with progesterone receptor

antagonist activity for use in contraceptive compns.)

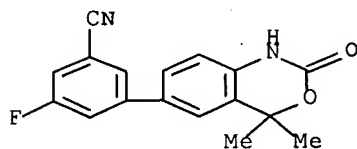
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CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



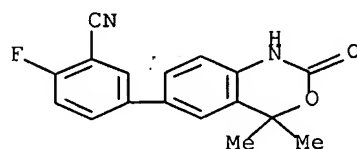
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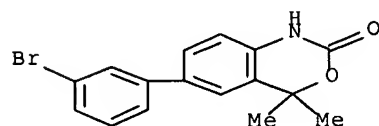
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RN 304854-49-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



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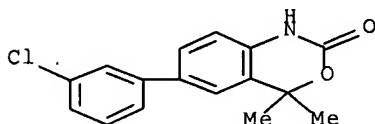
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted dihydrobenzoxazinones with progesterone receptor

antagonist activity for use in contraceptive compns.)

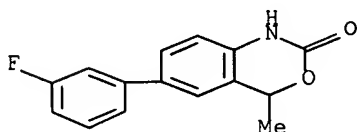
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CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
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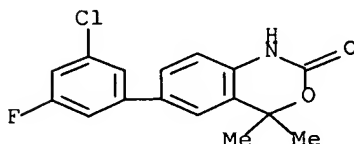
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 (CA INDEX NAME)



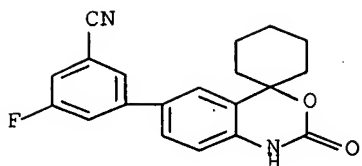
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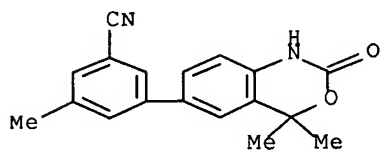
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CN Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



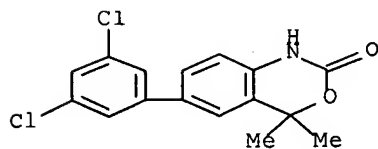
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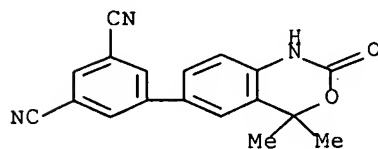
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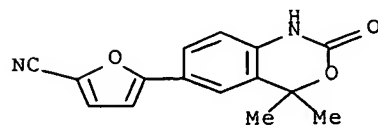
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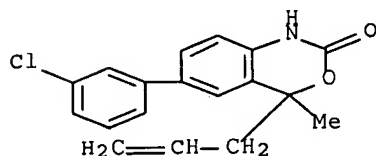
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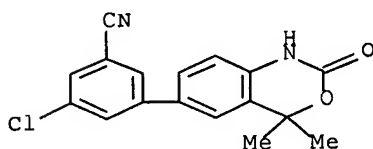
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CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(2-propenyl)- (9CI) (CA INDEX NAME)



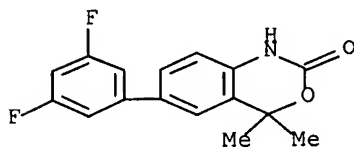
RN 304854-22-6 CAPLUS

CN Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



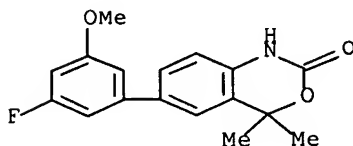
RN 304854-23-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3,5-difluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



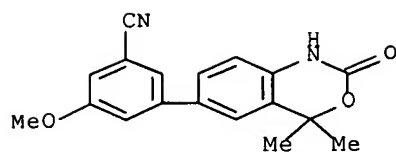
RN 304854-24-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



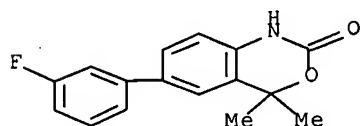
RN 304854-25-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-methoxy- (9CI) (CA INDEX NAME)



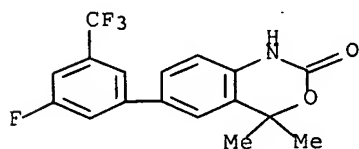
RN 304854-26-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



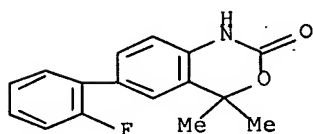
RN 304854-27-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(trifluoromethyl)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



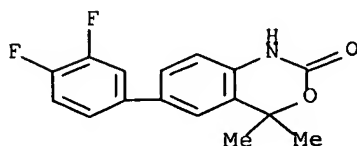
RN 304854-28-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2-fluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



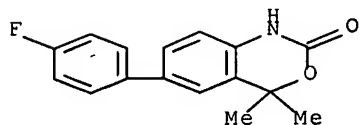
RN 304854-29-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3,4-difluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



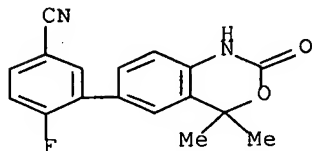
RN 304854-30-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(4-fluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



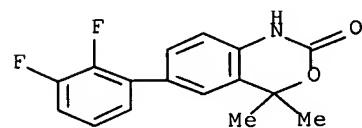
RN 304854-31-7 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro- (9CI) (CA INDEX NAME)



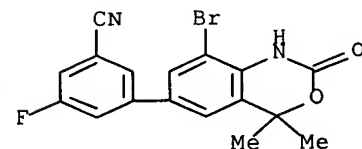
RN 304854-32-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2,3-difluorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



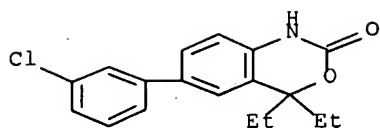
RN 304854-33-9 CAPLUS

CN Benzonitrile, 3-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



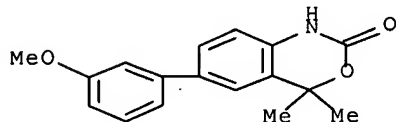
RN 304854-35-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4,4-diethyl-1,4-dihydro- (9CI)
(CA INDEX NAME)



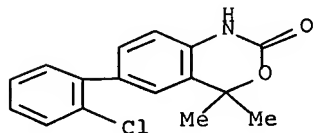
RN 304854-36-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-6-(3-methoxyphenyl)-4,4-dimethyl-
(9CI) (CA INDEX NAME)



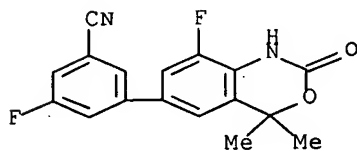
RN 304854-37-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(2-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
(9CI) (CA INDEX NAME)



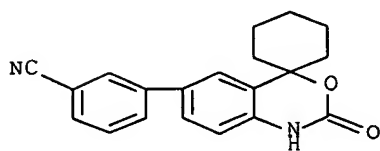
RN 304854-41-9 CAPLUS

CN Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



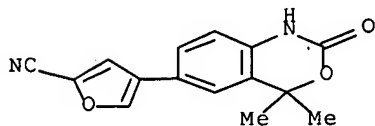
RN 304854-42-0 CAPLUS

CN Benzonitrile, 3-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)- (9CI) (CA INDEX NAME)



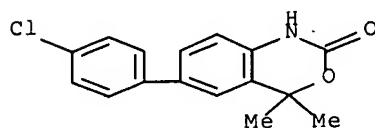
RN 304854-47-5 CAPLUS

CN 2-Furancarboxitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



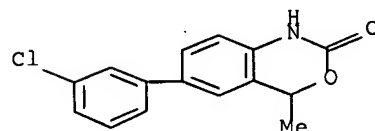
RN 305799-74-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(4-chlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



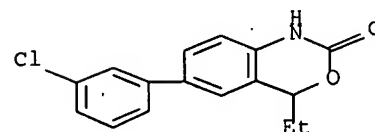
RN 305799-76-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)



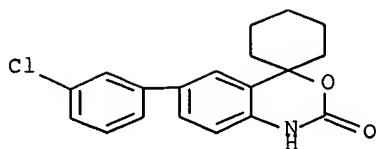
RN 305799-78-4 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethyl-1,4-dihydro- (9CI) (CA INDEX NAME)



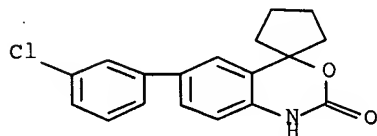
RN 305799-83-1 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one, 6-(3-chlorophenyl)- (9CI) (CA INDEX NAME)



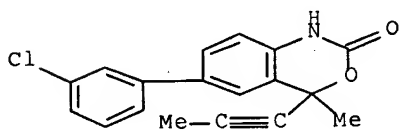
RN 305799-85-3 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-one, 6-(3-chlorophenyl)-
(9CI) (CA INDEX NAME)



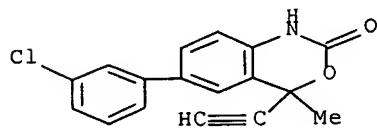
RN 305799-87-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(1-propynyl)- (9CI) (CA INDEX NAME)



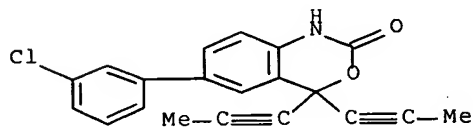
RN 305799-88-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethynyl-1,4-dihydro-4-methyl-
(9CI) (CA INDEX NAME)



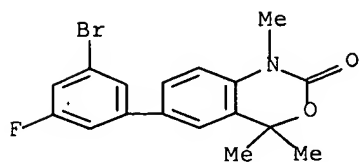
RN 305799-97-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-di-1-propynyl-
(9CI) (CA INDEX NAME)



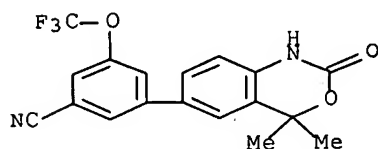
RN 305799-98-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-1,4,4-trimethyl- (9CI) (CA INDEX NAME)



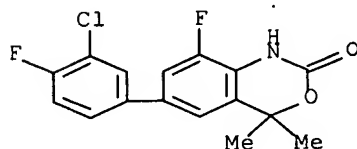
RN 305800-11-7 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



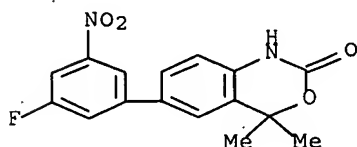
RN 305800-18-4 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-8-fluoro-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



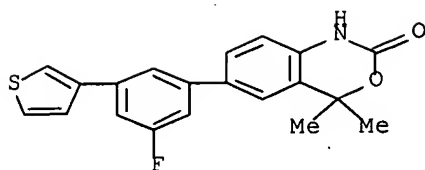
RN 305800-22-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-5-nitrophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



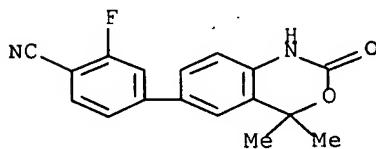
RN 305800-35-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(3-thienyl)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



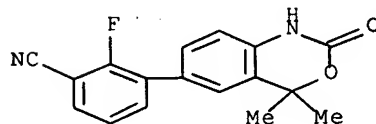
RN 305800-46-8 CAPLUS

CN Benzonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



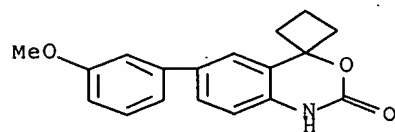
RN 305800-48-0 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



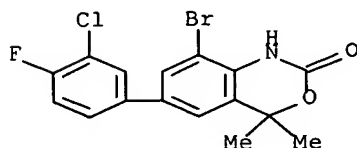
RN 305800-50-4 CAPLUS

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one, 6-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



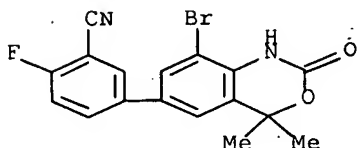
RN 305800-51-5 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 8-bromo-6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



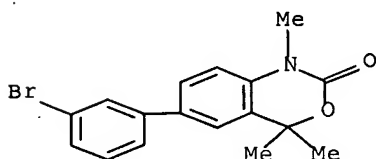
RN 305800-52-6 CAPLUS

CN Benzonitrile, 5-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



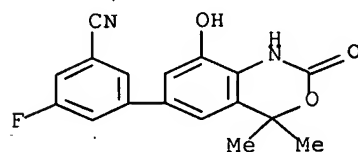
RN 305800-53-7 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-1,4,4-trimethyl- (9CI) (CA INDEX NAME)



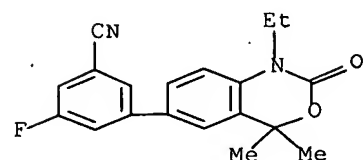
RN 305800-56-0 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-8-hydroxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



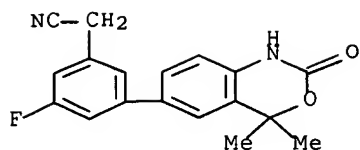
RN 305800-57-1 CAPLUS

CN Benzonitrile, 3-(1-ethyl-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



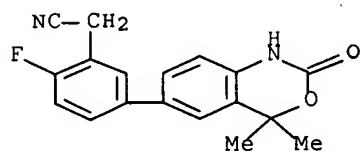
RN 305800-59-3 CAPLUS

CN Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



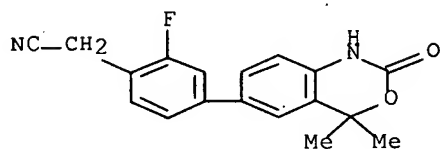
RN 305800-61-7 CAPLUS

CN Benzeneacetonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



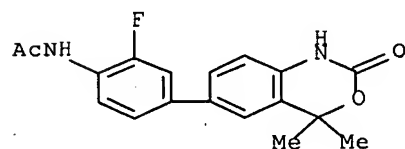
RN 305800-62-8 CAPLUS

CN Benzeneacetonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- (9CI) (CA INDEX NAME)



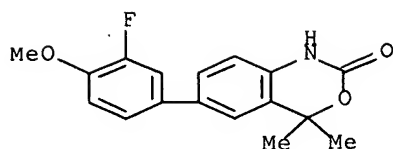
RN 305800-64-0 CAPLUS

CN Acetamide, N-[4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluorophenyl]- (9CI) (CA INDEX NAME)



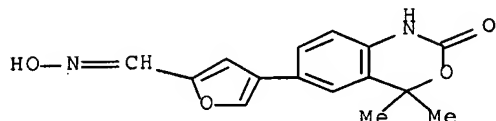
RN 305800-65-1 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-fluoro-4-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



RN 305800-72-0 CAPLUS

CN 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-, 2-oxime (9CI) (CA INDEX NAME)



IT 304853-36-9P 304854-10-2P 304854-11-3P

304854-45-3P 305800-55-9P 305800-70-8P

305800-71-9P

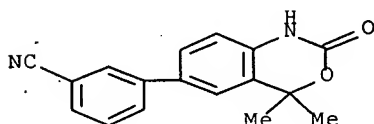
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted dihydrobenzoxazinones with progesterone receptor

antagonist activity for use in contraceptive compns.)

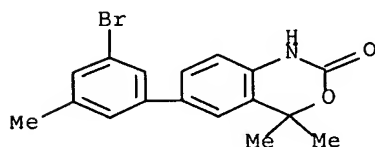
RN 304853-36-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



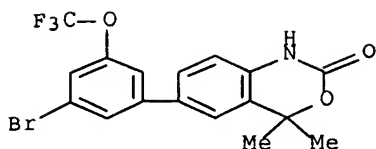
RN 304854-10-2 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-methylphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



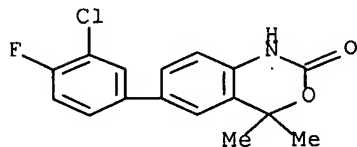
RN 304854-11-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[3-bromo-5-(trifluoromethoxy)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



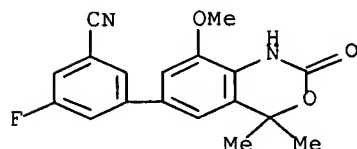
RN 304854-45-3 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



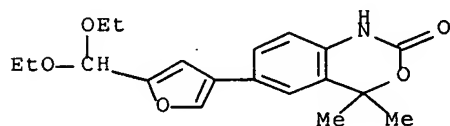
RN 305800-55-9 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-8-methoxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



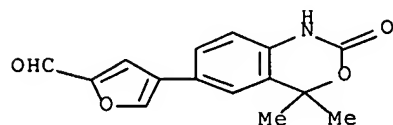
RN 305800-70-8 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[5-(diethoxymethyl)-3-furanyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)



RN 305800-71-9 CAPLUS

CN 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

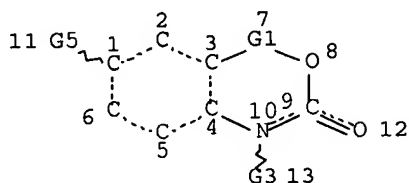
Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

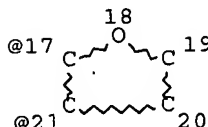
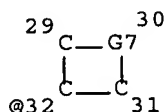
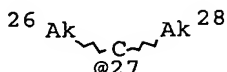
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L10

STR



Ak @14

Cb~G6
@15 16O~Ak
@22 23CH~Ak
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VAR G1=CH2/24/27/32

VAR G3=H/14

VAR G5=15/17/21

VAR G6=X/22/CN

REP G7=(0-5) C

NODE ATTRIBUTES:

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MLEVEL IS CLASS AT 14 15 23 25 26 28

GGCAT IS MCY LOC UNS AT 15

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

L13 78 SEA FILE=REGISTRY SSS FUL L10

100.0% PROCESSED 8380 ITERATIONS
SEARCH TIME: 00.00.01

78 ANSWERS

FILE 'CAPLUS' ENTERED AT 10:00:37 ON 12 SEP 2007
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FILE LAST UPDATED: 11 Sep 2007 (20070911/ED)

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L10 STR
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L24 13 SEA FILE=CAPLUS ABB=ON L13

L32 4 L24 NOT L25

=> fil chemcats; d que nos 127; fil marpat; d stat que 130
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For the list of current catalogs, enter HELP CTA, HELP CTBC, HELP CTDH, HELP CTIN, HELP CTOP, and HELP CTQZ.

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L27          11 SEA FILE=CHEMCATS ABB=ON  L13
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FILE 'MARPAT' ENTERED AT 10:01:02 ON 12 SEP 2007
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FILE CONTENT: 1961-PRESENT VOL 147 ISS 11 (20070907/ED)

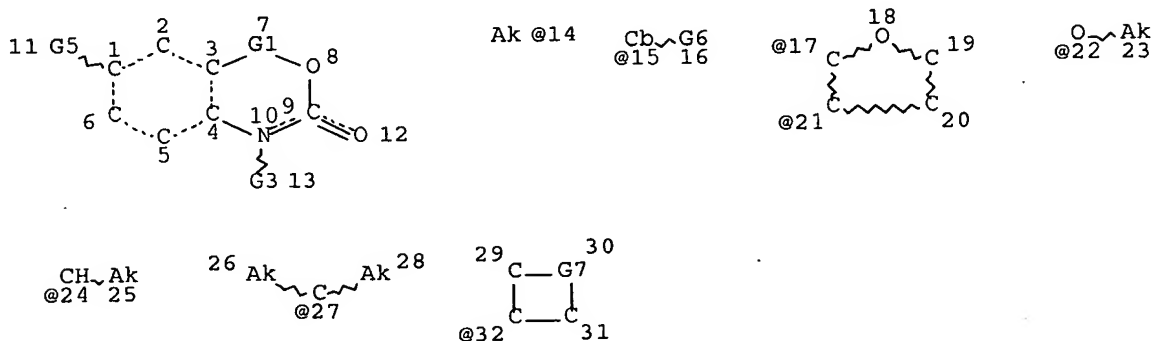
SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
 (COVERAGE TO THESE DATES IS NOT COMPLETE):

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US    2007173668 26 JUL 2007
DE 102006033242 26 JUL 2007
EP      1810967 25 JUL 2007
JP    2007189148 26 JUL 2007
WO    2007085204 02 AUG 2007
GB      2433499 27 JUN 2007
FR      2896409 27 JUL 2007
RU      2303603 27 JUL 2007
CA      2571093 16 JUN 2007
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Expanded G-group definition display now available.

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L10          STR
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VAR G1=CH2/24/27/32
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 VAR G5=15/17/21
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 2195 ITERATIONS
 SEARCH TIME: 00.00.02

12 ANSWERS

=> dup rem 132,130,127
 DUPLICATE IS NOT AVAILABLE IN 'CHEMCATS'.
 ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
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 PROCESSING COMPLETED FOR L32
 PROCESSING COMPLETED FOR L30
 PROCESSING COMPLETED FOR L27

L33 26 DUP REM L32 L30 L27 (1 DUPLICATE REMOVED)
 ANSWERS '1-4' FROM FILE CAPLUS
 ANSWERS '5-15' FROM FILE MARPAT
 ANSWERS '16-26' FROM FILE CHEMCATS

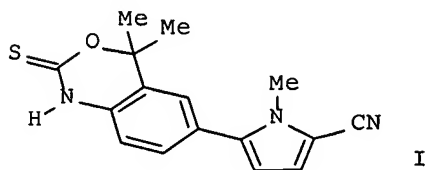
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L33 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 2005:1200915 CAPLUS Full-text
 DOCUMENT NUMBER: 143:460167
 TITLE: Purification of progesterone receptor modulators

INVENTOR(S): Wilk, Bodgan Kazimierz; Rubezhov, Arkadiy Zinovi; Hadfield, Anthony Francis; Helom, Jean Louise
 PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
 SOURCE: PCT Int. Appl., 39 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005104711	A2	20051110	WO 2005-US13997	20050425
WO 2005104711	A3	20061228		
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AU 2005237520	A1	20051110	AU 2005-237520	20050425
CA 2563063	A1	20051110	CA 2005-2563063	20050425
US 2005250766	A1	20051110	US 2005-113730	20050425
EP 1756072	A2	20070228	EP 2005-742297	20050425
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CN 1953967	A	20070425	CN 2005-80013278	20050425
IN 2006KN02984	A	20070608	IN 2006-KN2984	20061016
MX 2006PA12403	A	20070117	MX 2006-PA12403	20061026
PRIORITY APPLN. INFO.:				
			US 2004-565659P	P 20040427
			WO 2005-US13997	W 20050425

OTHER SOURCE(S): MARPAT 143:460167
 GI



AB Methods for purifying a compound compds. such as I include mixing the compound and a solvent; adding a base to the solvent; and precipitating purified compound E.g., I was purified via treatment with K tert-butoxide. Also salts of 5'-(5-cyano-1-methyl-1H-pyrrol-2-yl)spiro[cyclohexane-1,3'-[3H]indol]-2'-

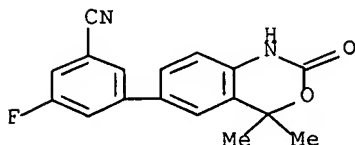
ylidenecyanamide such as Na, K, and choline were prepared and used to purify the base compound

IT 304853-30-3P 304854-22-6P 868862-31-1P

RL: PUR (Purification or recovery); PREP (Preparation)
(purification of progesterone receptor modulators)

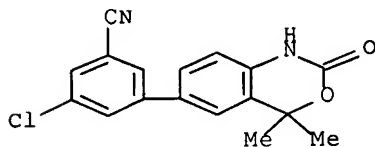
RN 304853-30-3 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



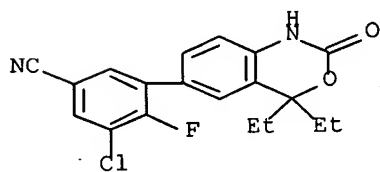
RN 304854-22-6 CAPLUS

CN Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)



RN 868862-31-1 CAPLUS

CN Benzonitrile, 3-chloro-5-(4,4-diethyl-1,4-dihydro-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro- (9CI) (CA INDEX NAME)



L33 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:709492 CAPLUS Full-text

DOCUMENT NUMBER: 145:225008

TITLE: Determination of conformational changes in the

progesterone receptor using ELISA-like assays

AUTHOR(S): Pullen, Mark A.; Laping, Nicholas; Edwards, Richard;
Bray, Jeffrey

CORPORATE SOURCE: Department of Urogenital Biology, GlaxoSmithKline
Pharmaceuticals, King of Prussia, PA, 19406, USA

SOURCE: Steroids (2006), 71(9), 792-798

CODEN: STEDAM; ISSN: 0039-128X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The conformation of proteins often influences their functional activity. The effect of progesterone receptor ligands on the C-terminal conformation of the progesterone receptor affects the recruitment of transcriptional cofactors. These conformations can be studied by differential sensitivity to proteolytic cleavage or immunopptn. with a conformation-specific antibody. This study describes an ELISA-like method using conformation-specific antibodies to the C-terminal or an area adjacent to the DNA binding region. Progesterone receptor ligands are shown to influence how the progesterone receptor interacts with these antibodies in a concentration dependent manner. This method allows for quick determination of the potency of agonists as well as mechanistic studies of antagonism. The conformation inducing activity of several standard agonist and antagonist compds. were compared to their binding affinity and ability to induce alkaline phosphatase in T47D cells. This method is useful for screening compds. for functional activity at the progesterone receptor and demonstrates that J 867 induces an antagonist conformation of the progesterone receptor similar to the antagonist RU486.

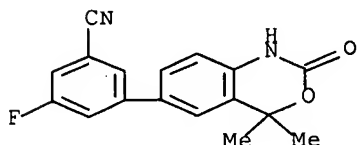
IT 304853-30-3, PRA 910

RL: ANT (Analyte); PAC (Pharmacological activity); ANST (Analytical study); BIOL (Biological study)

(progesterone receptor conformational change detection using ELISA-like assays in screening for agonists and antagonists)

RN 304853-30-3 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:493566 CAPLUS Full-text

DOCUMENT NUMBER: 143:43888

TITLE: Carbon-carbon cross coupling reactions catalyzed by

transition metals on solid supports

INVENTOR(S): Wilk, Bogdan Kazimierz

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: PCT Int. Appl., 22 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051869	A2	20050609	WO 2004-US39015	20041119
WO 2005051869	A3	20060406		

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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
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 NE, SN, TD, TG

AU 2004293427 A1 20050609 AU 2004-293427 20041119
 CA 2546352 A1 20050609 CA 2004-2546352 20041119
 EP 1687282 A2 20060809 EP 2004-811693 20041119

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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 HR, IS, YU

CN 1886387 A 20061227 CN 2004-80034589 20041119
 BR 2004016863 A 20070227 BR 2004-16863 20041119
 JP 2007520454 T 20070726 JP 2006-541563 20041119
 US 2005137438 A1 20050623 US 2004-994598 20041122
 IN 2006KN01235 A 20070427 IN 2006-KN1235 20060511
 NO 2006002192 A 20060822 NO 2006-2192 20060515
 MX 2006PA05640 A 20060817 MX 2006-PA5640 20060518

PRIORITY APPLN. INFO.: US 2003-524554P P 20031124
 WO 2004-US39015 W 20041119

OTHER SOURCE(S): CASREACT 143:43888

AB A method of coupling C-containing compds. comprises reaction of a first C-
 containing compound with a second C-containing compound in the presence of a
 Pd or Ni metal catalyst on a support comprising an alkaline earth metal salt
 in an alc. solvent. Thus, a mixture of 3-bromo-5-chlorobenzonitrile, 4,4-
 dimethyl-2-oxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-boronic acid, soda ash,
 and unreduced Pd/C in EtOH was heated at 80° overnight to give 63% 3-chloro-5-
 (4,4-dimethyl-2-oxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)benzonitrile.

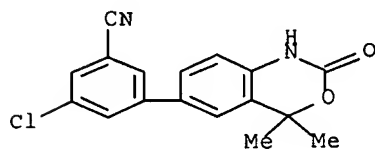
IT 304854-22-6P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)

(carbon-carbon cross coupling reactions catalyzed by transition metals
 on solid supports)

RN 304854-22-6 CAPLUS

CN Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-
 6-yl)- (9CI) (CA INDEX NAME)



L33 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:967696 CAPLUS Full-text

DOCUMENT NUMBER: 141:1442

TITLE: Regulation of gene expression by PRA-910, a novel
 progesterone receptor modulator, in T47D cells

AUTHOR(S): Bray, Jeffrey D.; Zhang, Zhiming; Winneker, Richard
 C.; Lyttle, C. Richard

CORPORATE SOURCE: Women's Health Research Institute, Wyeth Research,
 Collegeville, PA, 19426, USA

SOURCE: Steroids (2003), 68(10-13), 995-1003

CODEN: STEDAM; ISSN: 0039-128X

PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

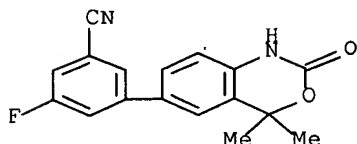
AB Progesterins play an important role in women's health and are used in oral contraception, hormone therapy, and treatment of reproductive disorders. The effects of progestins upon gene expression in breast epithelium are poorly understood. In an attempt to characterize the mol. mechanism of progestin action, we used a gene expression profiling approach to examine the action of a novel progestin in the T47D cell model, a human breast cancer cell line. PRA-910 is a novel, nonsteroidal progesterone receptor modulator (PRM) with species-specific activities identified in a screen for selective PRMs. To understand the mechanism of action for PRA-910 in T47D cells, we compared its gene regulation to progesterone (P4) and RU486 through Affymetrix U95A GeneChip anal. and TaqMan RT-PCR. PRA-910, P4, and RU486 regulated 50, 108, and 16 genes by threefold or greater vs. vehicle, resp., with 18 genes having similar regulation for P4 and PRA-910. These data confirm and extend previous findings for T47D cells. We also obtained time course, concentration-response, cyclohexamide sensitivity, and PR-specificity data for two progestin-regulated genes, ATP1A1 and CLDN8. Our data demonstrate that PRA-910 has a unique gene regulation profile distinct from both P4 and RU486. Further investigation of the underlying mechanism for these differences is ongoing.

IT 304853-30-3, PRA 910

RL: PAC (Pharmacological activity); BIOL (Biological study)
 (regulation of gene expression by PRA-910, a novel progesterone receptor modulator, in T47D cells)

RN 304853-30-3 CAPLUS

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 5 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 146:401992 MARPAT Full-text

TITLE: Preparation of heterocyclic amide derivatives as RXR agonists for the treatment of dyslipidemia, hypercholesterolemia and diabetes

INVENTOR(S): Lagu, Bharat; Lebedev, Rimma; Pio, Barbara

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 52pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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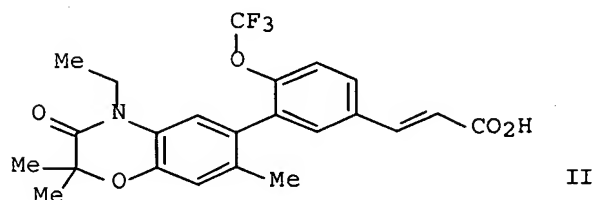
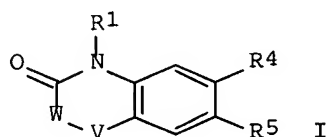
US 2007078129 A1 20070405 US 2006-534957 20060925
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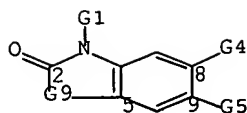
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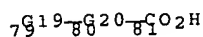


AB The present invention relates to compds. of formula I (wherein R1 is H or C1-3alkyl; W is -(O)-, -C(O)-, etc. ; V is -O-, substituted nitrogen, etc.; R4, R5 are H, (un)substituted alkyl, or ZXC02H where Z is alkoxy substituted Ph, thienyl, oxazolyl and X is a bond, (un)substituted alkoxy or (un)substituted alkylene), methods for preparing these compds., compns., intermediates and derivs. thereof and for treating RXR mediated disorders. More particularly, the compds. of the present invention are RXR agonists useful for treating RXR mediated disorders. Example compound II was prepared by converting 6-amino-m-cresol into a substituted 4H-benzo[1,4]oxazin-3-one by treatment with 2-bromoisobutyryl bromide. The 4H-benzo[1,4]oxazin-3-one was brominated and the amide nitrogen alkylated by a reaction with Et iodide. The resulting intermediate is reacted with an arylboronic acid to yield a benzaldehyde intermediate which is converted to II in two steps. In an ABCA1 bDNA assay and an RXR co-transfection assay, II had EC50's of 39.7 and 179.6 nM, resp.

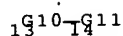
MSTR 1



G5 = 79



G9 = 13-2 14-5



G10 = O
G11 = 18



G17 = alkoxy <containing 1-3 C> (opt. substd.)

G19 = phenylene (opt. substd. by (1-3) G17)

G20 = bond

Patent location:

claim 1

Note:

substitution is restricted

L33 ANSWER 6 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:438652 MARPAT Full-text

TITLE: Preparation of compounds that modulate mitotic kinesin KSP and are useful against proliferative diseases and disorders

INVENTOR(S): Adams, Nicholas D.; Darcy, Michael Gerard; Dhanak, Dashyant; Duffy, Kevin J.; Fitch, Duke M.; Knight, Steven David; Newlander, Kenneth Allen; Shaw, Antony N.

PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 124pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006113432	A2	20061026	WO 2006-US14062	20060413
WO 2006113432	A3	20070712		

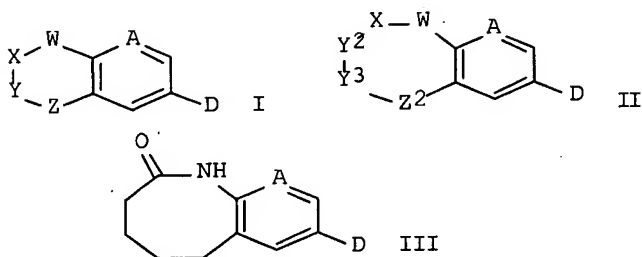
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,

MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
 SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
 VN, YU, ZA, ZM, ZW
 RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.:

US 2005-671299P 20050414

GI

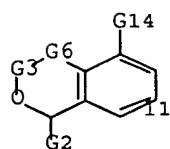


AB Compds. (shown as I, II and III; variables defined below; e.g. 6-[4-(trifluoromethyl)phenyl]-3,4-dihydro-1H-2,1,3-benzothiadiazine 2,2-dioxide (1)) useful for treating cellular proliferative diseases and disorders by modulating the activity of KSP are disclosed. Although the methods of preparation are not claimed, preps. and/or characterization data for .apprx.130 examples of I are included. For example, 1 was prepared in 3 steps starting with coupling of (4-trifluoromethylphenyl)boronic acid with 2-amino-5-bromobenzonitrile to give 60% 4-amino-4'-(trifluoromethyl)biphenyl-3-carbonitrile, which was reduced to 70% [3-(aminomethyl)-4'-(trifluoromethyl)biphenyl-4-yl]amine, which was cyclized with sulfamide (24%). For I-III: W is NR1, O, CH2, or CH(OH); R1 is H, C1-4alkyl, C1-4alkylaryl, CO2But, CO1-4alkyl, CH2CONMe2, or CO2CH2Ph; X is C:O, C:S, C:NOH, SO2, CH2, or CH(OH); Y-Z is V-CHR2; where V is O, NR3, or CHR4; R2 is H or C1-4alkyl; R3 is H, C1-2alkylOH, or C1-2alkyl; and R4 is H, C1-4alkyl, COSEt, NH2, OH, NHCHO, NHCOC1-4alkyl, NHSO2C1-4alkyl, CO2H, CH2OH, or CONH2; or Y-Z is V2:CR5, where V2 is N or OH; and R5 is H, Me or NH2; or Y-Z is V3-U, where V3 is CMe2, CO or CHR4. U is NR7, O, S, or SO2; R7 is H, CHO, or CH2R8, and R8 is H, CN, CO2Me, CONH2, CO2H, or CH2OH; or Y-Z is CH:N; A is N or CR10; R10 is H, F, CO2H, NH2, or NO2; D = 5-R12-6-R13pyridin-3-yl, 3-R11-4-R12-5-R13phenyl, or 4-R14cyclohex-1-enyl; R11 is H or F; R12 is H, halogen, Me, NH2, NHAc, NO2, CF3, 1-pyrrolyl, or CH2CN; R13 is H, CF3, CN, SO2CF3, SO2NMe2, SO2C1-3alkyl, SC1-3alkyl, halogen, 1-indolyl, Pri, But, NMe2 or NO2; or R12 and R13 taken together are OCF2O; and R14 is CF3 or C2-5alkyl; addnl. details including provisos are given in the claims. For II, in addition to the above definitions, Y2 is O, NR3, CHR4, or CMe2; Y3 is CH2, O, S, or NH; Z2 is CHR2, NR7, O, S, or SO2; or Y3-Z2 taken together is N:CH when Y2 is CHR4; addnl. details including provisos are given in the claims.

MSTR 1A

G1—G15

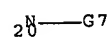
G1 = 11



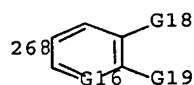
G3 = 14



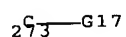
G4 = O
G6 = 20



G15 = 268



G16 = 273



G17 = F

Patent location:
Note:

claim 1
or pharmaceutically acceptable derivatives or
solvates

Note:

substitution is restricted

Note:

also incorporates claim 14

L33 ANSWER 7 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:171000 MARPAT Full-text

TITLE: Preparation of benzoxazinones and benzoxazinethiones as
mineralocorticoid receptor modulators

INVENTOR(S): Higuchi, Robert I.; Zhi, Lin; Adams, Mark E.; Liu,
Yan; Karanewsky, Donald S.

PATENT ASSIGNEE(S): Ligand Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

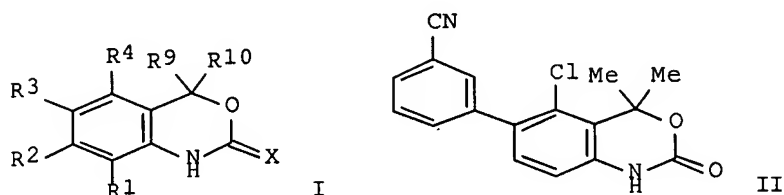
English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

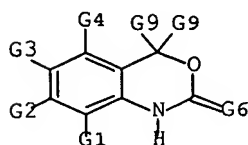
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006010142	A2	20060126	WO 2005-US24748	20050712
WO 2006010142	A3	20070104		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2007197520	A1	20070823	US 2007-622983	20070112
PRIORITY APPLN. INFO.:			US 2004-587947P	20040714
			WO 2005-US24748	20050712

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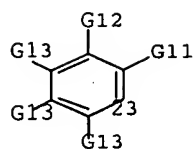


AB Title compds. I [R1 and R2 independently = F, Cl, CN. (un)substituted alkyl, etc.; R3 = (un)substituted aryl or heterocycle; R4 = H, halo, NO₂, etc.; R9 and R10 independently = H, (un)substituted alkyl, heteroalkyl, haloalkyl, etc.; X = O, S and NOR11 wherein R11 = H, (un)substituted alkyl, aryl, cycloalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as compds. that bind to mineralocorticoid receptors and/or modulate activity of mineralocorticoid receptors, and to methods for using such compds. Thus, e.g., II was prepared by coupling of 6-bromo-5-chloro-1,4-dihydro-4,4-dimethyl-2H-3,1-benzoxazin-2-one (preparation given) with 3-cyanophenylboronic acid. I were subjected to mineralocorticoid binding assays, e.g., II was determined to bind with a K_i value of 98.

MSTR 1



G3 = 23



G6 = O

G13 = F

Patent location:

claim 1

Note:

or pharmaceutically acceptable salts, esters, amides, or prodrugs

Note:

substitution is restricted

L33 ANSWER 8 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:81462 MARPAT Full-text

TITLE: Progesterone receptor antagonists, contraceptive regimens, and kits

INVENTOR(S): Grubb, Gary Sondermann; Constantine, Ginger Dale; Fensome, Andrew; McComas, Casey Cameron; Melenski, Edward George; Marella, Michael Anthony; Wrobel, Jay Edward

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: U.S. Pat. Appl. Publ., 22 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

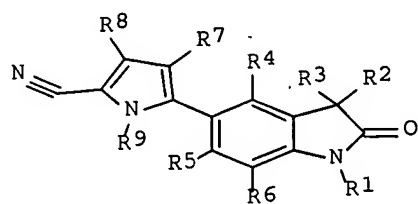
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006009509	A1	20060112	US 2005-175549	20050706
AU 2005271974	A1	20060216	AU 2005-271974	20050706
CA 2571198	A1	20060216	CA 2005-2571198	20050706
WO 2006017075	A1	20060216	WO 2005-US23798	20050706
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1773323	A1	20070418	EP 2005-771038	20050706
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1980660	A	20070613	CN 2005-80022750	20050706
KR 2007039912	A	20070413	KR 2007-700184	20070104
IN 2007DN00304	A	20070817	IN 2007-DN304	20070111
NO 2007000377	A	20070207	NO 2007-377	20070119
PRIORITY APPLN. INFO.:				
			US 2004-585883P	20040707
			US 2005-676135P	20050429
			WO 2005-US23798	20050706

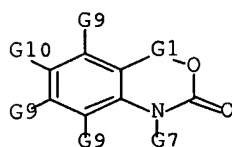
GI



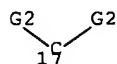
I

AB A method of contraception is provided which involves delivery of 21 to 27 consecutive days of one or more progesterone receptor (PR) antagonists in the absence of a progestin, estrogen, or other steroidal compound, followed by 1 to 7 days without any active agent. Also described is a pharmaceutically useful kit to facilitate delivery of this regimen. Example PR antagonists include mifepristone, onapristone, lilopristone, asoprisinyl, CDB-2914, substituted 1,4-dihydrobenzo[d][1,3]oxazin-2-ones, and carbonitriles of general formula I (wherein: R1 is H, (un)substituted alkyl, cycloalkyl, C3-C6 alkenyl, or C3-C6 alkynyl; R2 and R3 = H, (un)substituted alkyl; or R2 and R3 together form a ring; R4 = H or halogen; R5 = H; R6 = H or halogen; R7 = H, alkyl, or halogen; R8 = H; R9 = H, (un)substituted alkyl or COORA, where RA is alkyl or substituted alkyl).

MSTR 2



G1 = 17



G10 = 29

2G11-G12

G11 = phenylene (opt. substd. by (1-2) G16)

G12 = F

Patent location:

claim 2

Note:

substitution is restricted

Note:

additional oxo formation also claimed

Note:

or pharmaceutically acceptable salts

L33 ANSWER 9 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:386457 MARPAT Full-text

TITLE: Minimizing thioamide impurities during thionation of a cyano-containing carbonyl compound by using a nitrile decoy agent

INVENTOR(S): Wilk, Bogdan Kazimierz

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: U.S. Pat. Appl. Publ., 13 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005228179	A1	20051013	US 2005-100863	20050407
AU 2005233648	A1	20051027	AU 2005-233648	20050407
CA 2561313	A1	20051027	CA 2005-2561313	20050407
WO 2005100347	A1	20051027	WO 2005-US13657	20050407
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1732922	A1	20061220	EP 2005-738187	20050407
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1938298	A	20070328	CN 2005-80010293	20050407
BR 2005009213	A	20070828	BR 2005-9213	20050407
IN 2006KN02862	A	20070608	IN 2006-KN2862	20061004
MX 2006PA11695	A	20061214	MX 2006-PA11695	20061006
PRIORITY APPLN. INFO.: US 2004-560403P 20040408				
WO 2005-US13657 20050407				

AB A method is claimed for preventing, reducing or minimizing the formation of thioamide impurities (R7-C(:Y)-R8-R9-C(S)-NH₂) during thionation of a carbonyl compound (R7C(O)R8R9CN (I); variables defined below; e.g. 1-methyl-5-[2'-oxospiro[cyclohexane-1,3'-[3H]indole]-5'-yl]-1H-pyrrole-2- carbonitrile to the 2'-thioxo analog) comprising a nitrile group, comprising performing said thionation in the presence of a decoy agent comprising a nitrile group. For I: R7 is H, NH₂, NHR₁₀, N(R₁₀)₂, C(O)R₁₀, C(S)R₁₀, or (un)substituted C1 to C6 alkyl, C2 to C6 alkenyl, C2 to C6 alkynyl, C3 to C8 cycloalkyl, C1 to C6 thioalkyl, C1 to C6 alkoxy, aryl, or heteroaryl; R8 is (un)substituted C1 to C6 alkyl, C2 to C6 alkenyl, C2 to C6 alkynyl, C3 to C8 cycloalkyl, C1 to C6 alkoxy, aryl, or heteroaryl; or R7 and R8 are fused to form (un)saturated C-based 4 to 8 membered ring, 4 to 8 membered heterocyclic ring containing 1 to 3 heteroatoms O, N, and S; wherein rings are (un)substituted by 1 to 3 substituents H, or (un)substituted C1 to C6 alkyl, C2 to C6 alkenyl, C2 to C6 alkynyl, C3 to C8 cycloalkyl, C1 to C6 alkoxy, aryl, heteroaryl, or C1 to C6 aminoalkyl; R9 is absent, (un)substituted C1 to C6 alkyl, C2 to C6 alkenyl, C2 to C6 alkynyl, C3 to C8 cycloalkyl, C1 to C6 alkoxy, aryl, or heteroaryl; R₁₀ = H, or (un)substituted C1 to C6 alkyl, aryl, C1 to C6 alkoxy, C1 to C6

aminoalkyl, or C1 to C6 thioalkyl, NH₂, NHR₁₀, and N(R₁₁)₂; and R₁₁ = H, (un)substituted C1 to C6 alkyl, aryl, C1 to C6 alkoxy, C1 to C6 aminoalkyl, or C1 to C6 thioalkyl, or NH₂; Y = O, S. For example, use of MeCN as a decoy agent in a thionation of 5-(4,4-dimethyl-2-oxo-1,4-dihydrobenzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile by Lawesson's reagent resulted in 2.6 % thioamide impurity compared to 11-12 % when MeCN was absent.

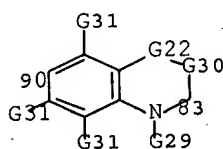
MSTR 1

G10 \Rightarrow G1

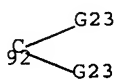
G1 = 0
G10 = 32

~~G15~~ ~~G14~~ ~~G16~~

G14 = arylene (opt. substd.)
G15 = 90-33 83-31



G16 = CN
G22 = 92



G30 = 0

Patent location:

claim 4

Note:

also incorporates claim 8

Note:

substitution is restricted

L33 ANSWER 10 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137:201317 MARPAT Full-text

TITLE: Preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents.

INVENTOR(S): Grubb, Gary S.; Zhang, Puwen; Terefenko, Eugene A.; Fensome, Andrew; Wrobel, Jay E.; Fletcher, Iii Horace; Edwards, James P.; Jones, Todd K.; Tegley, Christopher M.; Zhi, Lin

PATENT ASSIGNEE(S): Wyeth, John and Brother Ltd., USA; Ligand Pharmaceuticals Incorporated

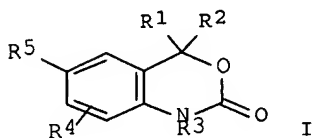
SOURCE: U.S., 44 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6444668	B1	20020903	US 2000-552350	20000419
CA 2372773	A1	20001109	CA 2000-2372773	20000501
JP 2002543155	T	20021217	JP 2000-615048	20000501
AT 275973	T	20041015	AT 2000-928611	20000501
PT 1173210	T	20050131	PT 2000-928611	20000501
ES 2226833	T3	20050401	ES 2000-928611	20000501
MX 2001PA11311	A	20030714	MX 2001-PA11311	20011105
US 2003045511	A1	20030306	US 2002-141792	20020509
US 6759408	B2	20040706		
HK 1043736	A1	20050401	HK 2002-104868	20020628

PRIORITY APPLN. INFO.:

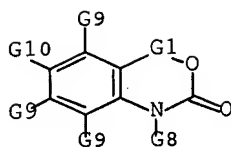
US 1999-229346P	19990504
US 1999-304712	19990504
US 2000-552350	20000419
WO 2000-US11643	20000501

GI



AB A method of contraception comprises administration to a female of a progestational agent in a first phase and in a second phase administration of [I; R1, R2 = H, (un)substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, aryl, heterocyclyl, amino derivative; R1R2 = atoms to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, C3-6 alkenyl, alkynyl, COR6; R6 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, alkynyl, C1-6 alkoxy, amino, C1-6 aminoalkyl; R5 = trisubstituted benzene ring, 5-6 membered ring with 1, 2, or 3 O, S, SO, SO2, NR7 and containing 1-2 H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, NR9COR8; R7 = H, C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl]. Thus, 6-(3-chlorophenyl)-4,4-dimethyl-1,4-dihydrobenzo[d][1,3]-oxazin-2-one was prepared from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. I demonstrated IC50's of 2.7-68 nM in a hPR decidualization assay.

MSTR 1



G1 = 13



G10 = 29

₂G11-G13

G11 = phenylene (opt. substd. by (1-2) G12)

G13 = F

Patent location:

claim 1

Note:

or pharmaceutically acceptable salts

REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 11 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 133:350229 MARPAT Full-text

TITLE: Novel cyclocarbamate derivatives as progesterone receptor modulators

INVENTOR(S): Zhang, Puwen; Terefenko, Eugene A.; Fletcher, Horace, III; Fensome, Andrew; Wrobel, Jay E.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.

PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 135 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

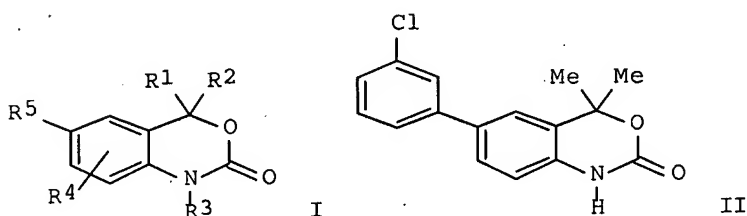
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066571	A1	20001109	WO 2000-US11822	20000501
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6509334	B1	20030121	US 2000-552633	20000419
CA 2371726	A1	20001109	CA 2000-2371726	20000501

EP 1173426	A1	20020123	EP 2000-928689	20000501
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010213	A	20020219	BR 2000-10213	20000501
TR 200103286	T2	20020722	TR 2001-3286	20000501
HU 200201609	A2	20020828	HU 2002-1609	20000501
JP 2002543193	T	20021217	JP 2000-615601	20000501
AU 766428	B2	20031016	AU 2000-46886	20000501
NZ 515355	A	20040227	NZ 2000-515355	20000501
SG 114650	A1	20050928	SG 2004-80	20000501
US 2002049204	A1	20020425	US 2001-948309	20010906
US 6566358	B2	20030520		
ZA 2001007630	A	20020514	ZA 2001-7630	20010917
IN 2001MN01295	A	20050318	IN 2001-MN1295	20011018
NO 2001005378	A	20020103	NO 2001-5378	20011102
NO 321361	B1	20060502		
BG 106079	A	20020531	BG 2001-106079	20011102
MX 2001PA11286	A	20030714	MX 2001-PA11286	20011105
US 2003216388	A1	20031120	US 2003-386799	20030312
US 6713478	B2	20040330		
US 2004186101	A1	20040923	US 2004-767813	20040129

PRIORITY APPLN. INFO.:

US 1999-183012P 19990504
US 2000-552633 20000419
WO 2000-US11822 20000501
US 2001-948309 20010906
US 2003-386799 20030312

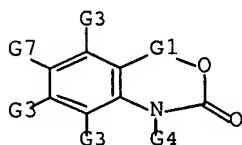
GI



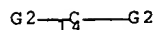
AB This invention discloses novel aryl fused cyclocarbamate derivs. I (R1 or R2 = H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, (un)substituted C3-8 cycloalkyl, (un)substituted aryl, (un)substituted heterocyclyl, amino derivative or R1 and R2 may be fused to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, (un)substituted C3-6 alkenyl, (un)substituted alkynyl, or COR6 {R6 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy, or (un)substituted C1-3 aminoalkyl}; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, (un)substituted alkynyl, (un)substituted C1-6 alkoxy, amino, or (un)substituted C1-6 aminoalkyl; R5 = trisubstituted benzene ring or a five- or six-membered ring with 1, 2, or 3 heteroatoms selected from O, S, SO, SO2 or NR7 and containing one or two independent substituents from the group including H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, or NR9COR8 {R7 = H or C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy or (un)substituted C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl}) or pharmaceutically acceptable salts thereof, as well as pharmaceutical compns. and methods using the compds. as antagonists of the progesterone receptor. Thus, cyclocarbamate II was prepared from 2-(2-amino-5-bromophenyl)propan-2-ol

via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. Compds. of the invention demonstrated potency in the range of 0.01 nM to 5 μ M in the in vitro assays, and 0.001 to 300 mg/kg in the in vivo assays.

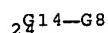
MSTR 1



G1 = 14



G7 = 24



G8 = F

G14 = phenylene (opt. substd. by (1-2) G9)

Patent location:

claim 1

Note:

substitution is restricted

Note:

or pharmaceutically acceptable salts

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 12 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 133:350205 MARPAT Full-text

TITLE: Contraceptive compositions containing antiprogesterinic and progestinic dihydro-2H-3,1-benzoxazin-2-ones

INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.

PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 146 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066164	A1	20001109	WO 2000-US11643	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,				

LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
 SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6498154	B1	20021224	US 2000-552357	20000419
CA 2372773	A1	20001109	CA 2000-2372773	20000501
EP 1173210	A1	20020123	EP 2000-928611	20000501
EP 1173210	B1	20040915		

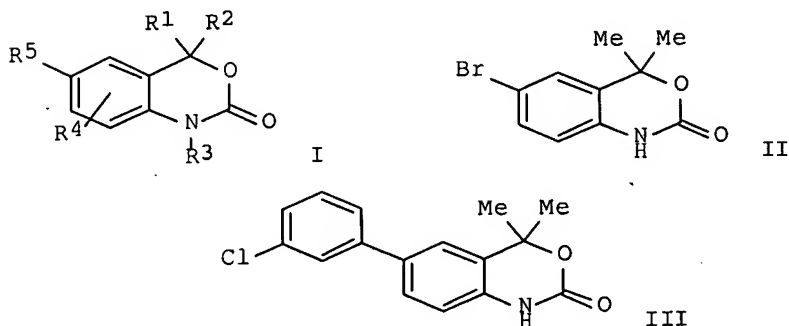
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO

JP 2002543155	T	20021217	JP 2000-615048	20000501
AT 275973	T	20041015	AT 2000-928611	20000501
TW 265032	B	20061101	TW 2000-89108477	20000725
MX 2001PA11311	A	20030714	MX 2001-PA11311	20011105
HK 1043736	A1	20050401	HK 2002-104868	20020628

PRIORITY APPLN. INFO.:

US 1999-304712	19990504
US 2000-552357	20000419
US 1999-183042P	19990504
US 2000-552350	20000419
WO 2000-US11643	20000501

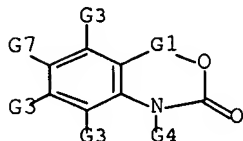
GI



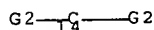
AB The dihydrobenzoxazinones I [R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, acyl, acylamino; or R1R2 are fused to form spirocyclic or hetero-spirocyclic rings substituted by F, alkyl, alkoxy, alkylthio, F3C, HO, cyano, H2N, alkylamino; R3 = H, OH, NH2, C1-6 alkyl, C3-6 alkenyl, alkynyl, CORC; RC = H, C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, cyano, NO2, alkyl, alkynyl, alkoxy, alkoxy, amino, aminoalkyl; R5 = XYZC6H2, X = halo, cyano, alkyl, alkenyl, alkynyl, alkoxy, thioalkoxy, H2N, aminoalkyl, NO2, perfluoroalkyl, 5- or 6-membered heterocyclyl; Y, Z = H, halo, cyano, NO2, H2N, aminoalkyl, alkoxy, alkyl, thioalkoxy; or R5 = 5- or 6-membered heterocyclyl with O, S, SO2 heteroatoms substituted by H, halo, cyano, NO2, H2N, alkyl, alkoxy, perfluoroacyl, perfluoroacylamino] and their pharmaceutically acceptable salts were prepared as antagonists of the progesterone receptor and were useful to induce contraception in mammals in cyclic combination therapies using an antiprogestin and progestin where the progestin is administered in the alternating presence and absence of an antiprogestin. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome,

carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects of cyclic menstrual bleeding. Addnl. uses of the invention include stimulation of food intake. Thus, cyclocondensation of 2-(2-amino-5-bromophenyl)-2-propanol with carbonyldiimidazole gave the dimethylbenzoxazinone II which coupled with 3-chlorophenylboronic acid in DME/H₂O containing (Ph₃P)₄Pd and Na₂CO₃ to give the (chlorophenyl)benzoxazinone III.

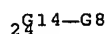
MSTR 1



G1 = 14



G7 = 24



G8 = F

G14 = phenylene (opt. substd. by (1-2) G9)

Patent location: claim 1

Note: substitution is restricted

Note: or pharmaceutically acceptable salts

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 13 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 133:330061 MARPAT Full-text

TITLE: Cyclic regimens using cyclic urea and cyclic amide derivatives

INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Tegley, Christopher M.; Puwen, Zhang; Fensome, Andrew; Viet, Andrew Q.; Santilli, Arthur A.; Terefenko, Eugene A.; Wrobel, Jay E.; Edwards, James P.

PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 61 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2000066103	A2	20001109	WO 2000-US11449	20000501
WO 2000066103	A3	20010405		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
 CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
 ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
 LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
 SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6399593	B1	20020604	US 2000-552037	20000419
CA 2372768	A1	20001109	CA 2000-2372768	20000501
EP 1173208	A2	20020123	EP 2000-928519	20000501

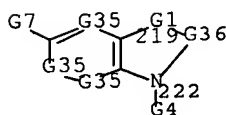
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO

JP 2002543119	T	20021217	JP 2000-614988	20000501
MX 2001PA11307	A	20030714	MX 2001-PA11307	20011105

PRIORITY APPLN. INFO.:
 US 1999-198238P 19990504
 US 2000-552037 20000419
 WO 2000-US11449 20000501

AB This invention concerns cyclic combination therapies using indoline derivs., which are progesterone receptor antagonists, or a pharmaceutically acceptable salt thereof. These methods may be used for contraception or treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects or cyclic menstrual bleeding. Addnl. uses of the invention include stimulation of food intake. For example, 6-(3-chlorophenyl)-4,4-dimethyl-1,4-dihydro-3-oxa-1,8-diaza-naphthalene-2-one was prepared and tested in the range of 0.01 nM to 5 μ M in the in vitro assays and 0.001-300 mg/kg in the in vivo assays.

MSTR 1



G1 = 14

G2— C_4 —G2

G7 = 24

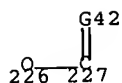
2G^{14} —G8

G8 = F

G14 = phenylene (opt. substd. by (1-2) G9)

G35 = CH

G36 = 226-219 227-222



G42 = O

Patent location:

claim 1.

Note:

substitution is restricted

Note:

or pharmaceutically acceptable salts

L33 ANSWER 14 OF 26 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 130:196659 MARPAT Full-text

TITLE: Preparation of 4,4-disubstituted-1,4-dihydro-2H-3,1-benzoxazin-2-ones and related compounds useful as HIV reverse transcriptase inhibitors.

INVENTOR(S): Christ, David Donald; Cocuzza, Anthony Joseph; Ko, Soo Sung; Markwalder, Jay Andrew; Mutlib, Abdul Ezaz; Parsons, Rodney Lawrence, Jr.; Patel, Mona; Seitz, Steven Paul

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: U.S., 74 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

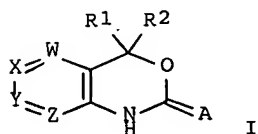
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5874430	A	19990223	US 1997-942031	19971001
US 6140499	A	20001031	US 1998-176491	19981021
US 6303780	B1	20011016	US 2000-627213	20000727
US 2002040138	A1	20020404	US 2001-919065	20010731
US 6492515	B2	20021210		
PRIORITY APPLN. INFO.:			US 1996-27137P	19961002
			US 1997-45138P	19970430
			US 1997-942031	19971001
			US 1998-176491	19981021
			US 2000-627213	20000727

OTHER SOURCE(S): CASREACT 130:196659

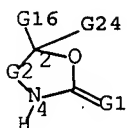
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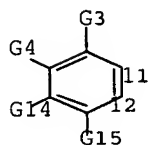
AB Title compds. [I; A = O, S; W = N, CR3; X = N, CR4; Y = N, CR5; Z = N, CR6; Q = O, S, NH; R1 = CF3, CF2H, C2F5, alkyl, cycloalkyl, alkenyl, alkynyl; R2 = QCHR7R8, QCHR7C.tplbond.CR8, QCHR7C:CR8, Q(CH2)pCHR7R8, C.tplbond.CR8,

CH:CR7R8, (CH2)pCHR7R8, CHR7C.tplbond.CR8, CHR7CH:CHR8, CH:CHCHR7R8; R3 = H, F, Cl, Br, iodo, alkoxy, alkyl; R4 = H, F, Cl, Br, iodo, (substituted) alkyl, alkenyl, alkynyl, alkoxy, OCF3, cyano, NO2, CHO, Ac, COCF3, CONH2, CONHMe, NR7R7a, NR7CO2R7a, CO2R7, SOpR7, SO2NHR7, NR7SO2R7b, Ph, heteroaryl; R3R4 = OCH2O; R5 = H, F, Cl, Br, iodo; R4R5 = OCH2O, fused benzo ring; R6 = H, OH, alkoxy, cyano, F, Cl, Br, iodo, NO2, CF3, CHO, alkyl, CONH2; R7, R7a = H, alkyl; R8 = H, (substituted) alkyl, CH(OCH2CH2O), alkenyl, cycloalkyl, Ph, heteroaryl; p = 0-2; with provisos], were prepared for treatment of HIV infection (no data). Thus, 5-chloro-1-pentyne in THF at 0° was treated with BuLi; the mixture was warmed to room temperature, cooled to -20°, and treated with 2'-amino-5'-chloro-3'-(tert-butyldimethylsilyloxy)-2,2,2-trifluoroacetophenone (preparation given) in THF followed by 30 min. stirring to give 70% 2-[2-amino-5-chloro-3-(tert-butyldimethylsilyloxy)phenyl]-4-cyclopropyl-1,1,1-trifluoro-3-butyn-2-ol. The latter in PhMe was treated with (Me2CH)2NEt and COCl2 at -25° to give a residue which was treated with Bu4NF in THF to give 94% 6-chloro-4-(cyclopropylethynyl)-8-hydroxy-4-trifluoromethyl-1,4-dihydro-2H-3,1-benzoxazin-2-one.

MSTR 1



G1 = O
G2 = 11-2 12-4

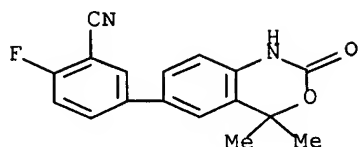


G4 = carbocycle <containing 6 C, aromatic, bonds all normalized, 6-membered monocyclic ring> (opt. substd. by (1-2) G13)
G13 = F
G16 = alkyl <containing 1-4 C>
G19 = carbon chain <0 or more double bonds, 0 or more triple bonds>
G24 = 161

1G19-1G17

Derivative: or pharmaceutically acceptable salts
Patent location: claim 1
Note: substitution is restricted
Stereochemistry: or stereoisomers

CAS Registry No. (RN): 304854-07-7
Structure :



PRICES

Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

Milestone PharmTech LLC
100 Jersey Ave. Building D, Box D-4
New Brunswick, NJ, 08901
USA

Phone: 1-732-579-8201

Fax: 1-732-653-0236

Fax: 1-732-579-8252

Email: services@milestonepharmtech.com

Web: <http://www.milestonepharmtech.com>

L33 ANSWER 17 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2025595856 CHEMCATS

Catalog Name (CO): Milestone PharmTech Product List

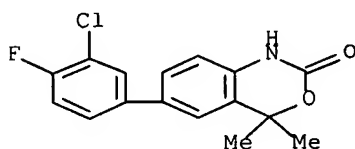
Publication Date (PD): 27 Mar 2007

Order Number (ON): 5B-0007

Chemical Name (CN): 6-(3-chloro-4-fluorophenyl)-4,4-dimethyl-1H-benzo[d][1,3]oxazin-2(4H)-one

CAS Registry No. (RN): 304854-45-3

Structure :



PRICES

Quantity : N/A, Price: contact supplier

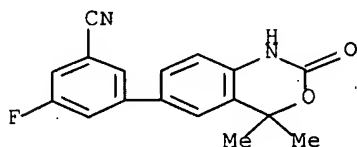
COMPANY INFORMATION

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USA

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Fax: 1-732-653-0236
Fax: 1-732-579-8252
Email: services@milestonepharmtech.com
Web: <http://www.milestonepharmtech.com>

L33 ANSWER 18 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
Accession No. (AN): 2025595855 CHEMCATS
Catalog Name (CO): Milestone PharmTech Product List
Publication Date (PD): 27 Mar 2007
Order Number (ON): 5B-0008
Chemical Name (CN): 3-(4,4-dimethyl-2-oxo-2,4-dihydro-1H-benzo[d][1,3]oxazin-6-yl)-5-fluorobenzonitrile
CAS Registry No. (RN): 304853-30-3
Structure :



PRICES

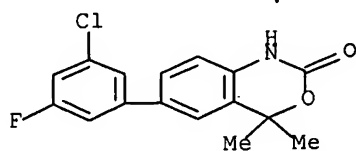
Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

Milestone PharmTech LLC
100 Jersey Ave. Building D, Box D-4
New Brunswick, NJ, 08901
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Phone: 1-732-579-8201
Fax: 1-732-653-0236
Fax: 1-732-579-8252
Email: services@milestonepharmtech.com
Web: <http://www.milestonepharmtech.com>

L33 ANSWER 19 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
Accession No. (AN): 2025595854 CHEMCATS
Catalog Name (CO): Milestone PharmTech Product List
Publication Date (PD): 27 Mar 2007
Order Number (ON): 5B-0009
Chemical Name (CN): 6-(3-chloro-5-fluorophenyl)-4,4-dimethyl-1H-benzo[d][1,3]oxazin-2(4H)-one
CAS Registry No. (RN): 304854-09-9
Structure :



PRICES

Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

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Fax: 1-732-579-8252

Email: services@milestonepharmtech.com

Web: <http://www.milestonepharmtech.com>

L33 ANSWER 20 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2025595853 CHEMCATS

Catalog Name (CO): Milestone PharmTech Product List

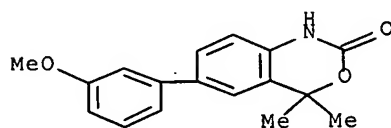
Publication Date (PD): 27 Mar 2007

Order Number (ON): 5B-0010

Chemical Name (CN): 6-(3-methoxyphenyl)-4,4-dimethyl-1H-benzo[d][1,3]oxazin-2(1H)-one

CAS Registry No. (RN): 304854-36-2

Structure :



PRICES

Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

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New Brunswick, NJ, 08901
USA

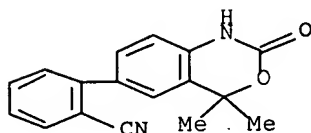
Phone: 1-732-579-8201

Fax: 1-732-653-0236

Fax: 1-732-579-8252

Email: services@milestonepharmtech.com
 Web: <http://www.milestonepharmtech.com>

L33 ANSWER 21 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
 Accession No. (AN): 2025595852 CHEMCATS
 Catalog Name (CO): Milestone PharmTech Product List
 Publication Date (PD): 27 Mar 2007
 Order Number (ON): 5B-0011
 Chemical Name (CN): 2-(4,4-dimethyl-2-oxo-2,4-dihydro-1H-benzo[d][1,3]oxazin-6-yl)benzonitrile
 CAS Registry No. (RN): 885268-52-0
 Structure :



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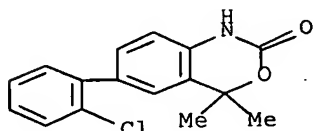
Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

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L33 ANSWER 22 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
 Accession No. (AN): 2025595851 CHEMCATS
 Catalog Name (CO): Milestone PharmTech Product List
 Publication Date (PD): 27 Mar 2007
 Order Number (ON): 5B-0012
 Chemical Name (CN): 6-(2-chlorophenyl)-4,4-dimethyl-1H-benzo[d][1,3]oxazin-2(4H)-one
 CAS Registry No. (RN): 304854-37-3
 Structure :



PRICES

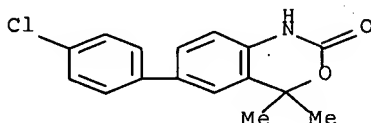
Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

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Web: <http://www.milestonepharmtech.com>

L33 ANSWER 23 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
Accession No. (AN): 2025595850 CHEMCATS
Catalog Name (CO): Milestone PharmTech Product List
Publication Date (PD): 27 Mar 2007
Order Number (ON): 5B-0013
Chemical Name (CN): 6-(4-chlorophenyl)-4,4-dimethyl-1H-benzo[d][1,3]oxazin-2(4H)-one
CAS Registry No. (RN): 305799-74-0
Structure :



PRICES

Quantity : N/A, Price: contact supplier

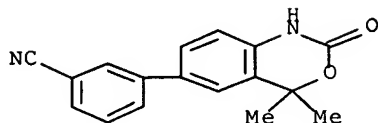
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L33 ANSWER 24 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
Accession No. (AN): 2025595849 CHEMCATS
Catalog Name (CO): Milestone PharmTech Product List
Publication Date (PD): 27 Mar 2007

Order Number (ON): 5B-0014
 Chemical Name (CN): 3-(4,4-dimethyl-2-oxo-2,4-dihydro-1H-benzo[d][1,3]oxazin-6-yl)benzonitrile
 CAS Registry No. (RN): 304853-36-9
 Structure :



PRICES

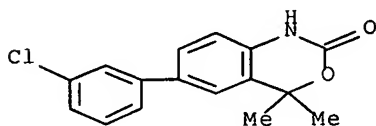
Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

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L33 ANSWER 25 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
 Accession No. (AN): 2025595848 CHEMCATS
 Catalog Name (CO): Milestone PharmTech Product List
 Publication Date (PD): 27 Mar 2007
 Order Number (ON): 5B-0015
 Chemical Name (CN): 6-(3-Chlorophenyl)-4,4-dimethyl-1H-benzo[d][1,3]oxazin-2(4H)-one
 CAS Registry No. (RN): 304853-28-9
 Structure :



PRICES

Quantity : N/A, Price: contact supplier

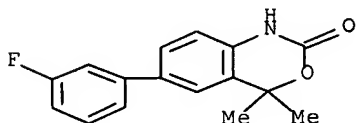
COMPANY INFORMATION

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L33 ANSWER 26 OF 26 CHEMCATS COPYRIGHT 2007 ACS on STN
Accession No. (AN): 2025595847 CHEMCATS
Catalog Name (CO): Milestone PharmTech Product List
Publication Date (PD): 27 Mar 2007
Order Number (ON): 5B-0016
Chemical Name (CN): 6-(3-fluorophenyl)-4,4-dimethyl-1H-
benzo[d][1,3]oxazin-2(4H)-one
CAS Registry No. (RN): 304854-26-0
Structure :



PRICES

Quantity : N/A, Price: contact supplier

COMPANY INFORMATION

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SPECIES

=> fil reg; d ide l5

FILE 'REGISTRY' ENTERED AT 10:02:23 ON 12 SEP 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 SEP 2007 HIGHEST RN 946658-01-1

DICTIONARY FILE UPDATES: 11 SEP 2007 HIGHEST RN 946658-01-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 305800-59-3 REGISTRY

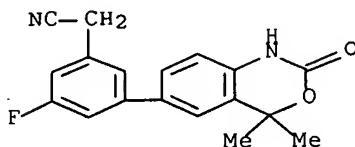
ED Entered STN: 01 Dec 2000

CN Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)

MF C18 H15 F N2 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil capl; s l5

FILE 'CAPLUS' ENTERED AT 10:02:30 ON 12 SEP 2007

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FILE COVERS 1907 - 12 Sep 2007 VOL 147 ISS 12
FILE LAST UPDATED: 11 Sep 2007 (20070911/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L34 3 L5

=> d scan ti

L34 3 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN
TI Contraceptive compositions containing antiprogesteric and progestinic dihydro-2H-3,1-benzoxazin-2-ones

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

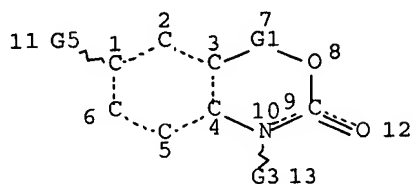
L34 3 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN
TI Novel cyclocarbamate derivatives as progesterone receptor modulators

L34 3 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN
TI Preparation of benzoxazinone cyclic carbamate antiprogesterins for use in combination therapies and regimens with progestational agents.

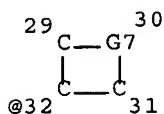
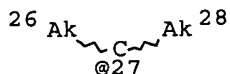
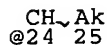
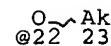
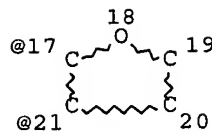
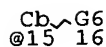
ALL ANSWERS HAVE BEEN SCANNED

SEARCH HISTORY

=> d stat que l13; d his nofile
L10 STR



Ak @14



VAR G1=CH2/24/27/32

VAR G3=H/14

VAR G5=15/17/21

VAR G6=X/22/CN

REP G7=(0-5) C

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 14

CONNECT IS E1 RC AT 23

CONNECT IS E1 RC AT 25

CONNECT IS E1 RC AT 26

CONNECT IS E1 RC AT 28

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 14 15 23 25 26 28

GGCAT IS MCY LOC UNS AT 15

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

L13 78 SEA FILE=REGISTRY SSS FUL L10

100.0% PROCESSED 8380 ITERATIONS
SEARCH TIME: 00.00.01

78 ANSWERS

(FILE 'HOME' ENTERED AT 09:35:14 ON 12 SEP 2007)

FILE 'CAPLUS' ENTERED AT 09:35:32 ON 12 SEP 2007

E US2004-767813/APPS

L1 1 SEA ABB=ON US2004-767813/AP
D SCAN
SEL RN

FILE 'REGISTRY' ENTERED AT 09:35:57 ON 12 SEP 2007

L2 250 SEA ABB=ON (100-58-3/BI OR 10365-98-7/BI OR 105942-08-3/BI OR
1066-54-2/BI OR 1072-85-1/BI OR 1072-97-5/BI OR 1073-06-9/BI

OR 108-36-1/BI OR 110-52-1/BI OR 111-24-0/BI OR 112575-11-8/BI
 OR 114897-91-5/BI OR 1191-95-3/BI OR 121359-48-6/BI OR
 122-51-0/BI OR 130723-13-6/BI OR 13331-27-6/BI OR 135884-31-0/B
 I OR 141940-30-9/BI OR 14282-76-9/BI OR 1435-51-4/BI OR
 145543-82-4/BI OR 149947-15-9/BI OR 154598-53-5/BI OR 1546-79-8
 /BI OR 160892-07-9/BI OR 1611-92-3/BI OR 161957-56-8/BI OR
 1679-18-1/BI OR 1730-25-2/BI OR 179897-89-3/BI OR 179898-34-1/B
 I OR 18242-39-2/BI OR 18791-99-6/BI OR 18792-00-2/BI OR
 188813-02-7/BI OR 189331-47-3/BI OR 19472-74-3/BI OR 206551-41-
 9/BI OR 207226-31-1/BI OR 21440-97-1/BI OR 21440-99-3/BI OR
 2160-62-5/BI OR 216755-56-5/BI OR 216755-57-6/BI OR 2357-52-0/B
 I OR 27065-51-6/BI OR 29578-39-0/BI OR 304853-28-9/BI OR
 304853-29-0/BI OR 304853-30-3/BI OR 304853-31-4/BI OR 304853-36
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 304854-54-4/BI OR 304854-55-5/BI OR 304854-57-7/BI OR 304

L3 83 SEA ABB=ON L2 AND F/ELS
 L4 26 SEA ABB=ON L3 AND N>1
 D SCAN
 E BENZENEACETONITRILE, 3-(1,4-DIHYDRO-4,4-DIMETHYL-2-OXO-2H-3,
 L5 1 SEA ABB=ON "BENZENEACETONITRILE, 3-(1,4-DIHYDRO-4,4-DIMETHYL-2
 -OXO-2H-3,1-BENZOXAZIN-6-YL)-5-FLUORO-"/CN
 D SCAN
 STR
 L6
 L7 4 SEA SSS SAM L6
 D SCAN
 L8 53 SEA ABB=ON L2 AND O>2
 L9 37 SEA ABB=ON L8 AND NR>2
 L10 STR L6
 L11 3 SEA SSS SAM L10
 L12 8380 SEA SSS FUL L10 EXTEND
 L13 78 SEA SSS FUL L10
 SAVE TEMP L13 BET813FULL/A
 L14 1 SEA ABB=ON L13 AND L5

FILE 'STNGUIDE' ENTERED AT 09:51:05 ON 12 SEP 2007

FILE 'CAPLUS' ENTERED AT 09:52:17 ON 12 SEP 2007

L15 7953 SEA ABB=ON ZHANG P?/AU
 L16 40 SEA ABB=ON TEREFEFENKO E?/AU
 L17 72 SEA ABB=ON FENSOME A?/AU
 L18 634 SEA ABB=ON WROBEL J?/AU
 L19 406 SEA ABB=ON FLETCHER H?/AU
 L20 245 SEA ABB=ON ZHI L?/AU
 L21 3830 SEA ABB=ON JONES T?/AU

L22 3382 SEA ABB=ON EDWARDS J?/AU
 L23 55 SEA ABB=ON TEGLEY C?/AU
 L24 13 SEA ABB=ON L13
 L25 9 SEA ABB=ON (L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR L21 OR
 L22 OR L23 OR L1) AND L24

L26 FILE 'REGISTRY' ENTERED AT 09:53:53 ON 12 SEP 2007
 ANALYZE L13 1- LC : 7 TERMS
 D

L27 FILE 'CHEMCATS' ENTERED AT 09:54:14 ON 12 SEP 2007
 11 SEA ABB=ON L13

L28 FILE 'MARPAT' ENTERED AT 09:54:26 ON 12 SEP 2007
 2 SEA SSS SAM L10
 D SCAN
 L29 2195 SEA SSS FUL L10 EXTEND
 L30 12 SEA SSS FUL L10
 SAVE TEMP L30 BET813MARPA

L31 FILE 'CAPLUS, MARPAT' ENTERED AT 09:56:14 ON 12 SEP 2007
 16 DUP REM L25 L30 (5 DUPLICATES REMOVED)
 ANSWERS '1-9' FROM FILE CAPLUS
 ANSWERS '10-16' FROM FILE MARPAT

FILE 'STNGUIDE' ENTERED AT 09:56:49 ON 12 SEP 2007

FILE 'CAPLUS' ENTERED AT 09:59:31 ON 12 SEP 2007
 D QUE NOS L25
 D IBIB ABS HITSTR L25 1-9

FILE 'REGISTRY' ENTERED AT 10:00:37 ON 12 SEP 2007
 D STAT QUE L13

L32 FILE 'CAPLUS' ENTERED AT 10:00:37 ON 12 SEP 2007
 D QUE NOS L24
 4 SEA ABB=ON L24 NOT L25

FILE 'CHEMCATS' ENTERED AT 10:01:02 ON 12 SEP 2007
 D QUE NOS L27

FILE 'MARPAT' ENTERED AT 10:01:02 ON 12 SEP 2007
 D STAT QUE L30

L33 FILE 'CAPLUS, MARPAT, CHEMCATS' ENTERED AT 10:01:14 ON 12 SEP 2007
 26 DUP REM L32 L30 L27 (1 DUPLICATE REMOVED)
 ANSWERS '1-4' FROM FILE CAPLUS
 ANSWERS '5-15' FROM FILE MARPAT
 ANSWERS '16-26' FROM FILE CHEMCATS
 D IBIB ABS HITSTR 1-4
 D IBIB ABS QHIT 5-15
 D ALL 16-26

FILE 'REGISTRY' ENTERED AT 10:02:23 ON 12 SEP 2007
 D IDE L5

L34 FILE 'CAPLUS' ENTERED AT 10:02:30 ON 12 SEP 2007
 3 SEA ABB=ON L5
 D SCAN TI
 D STAT QUE L13

=>